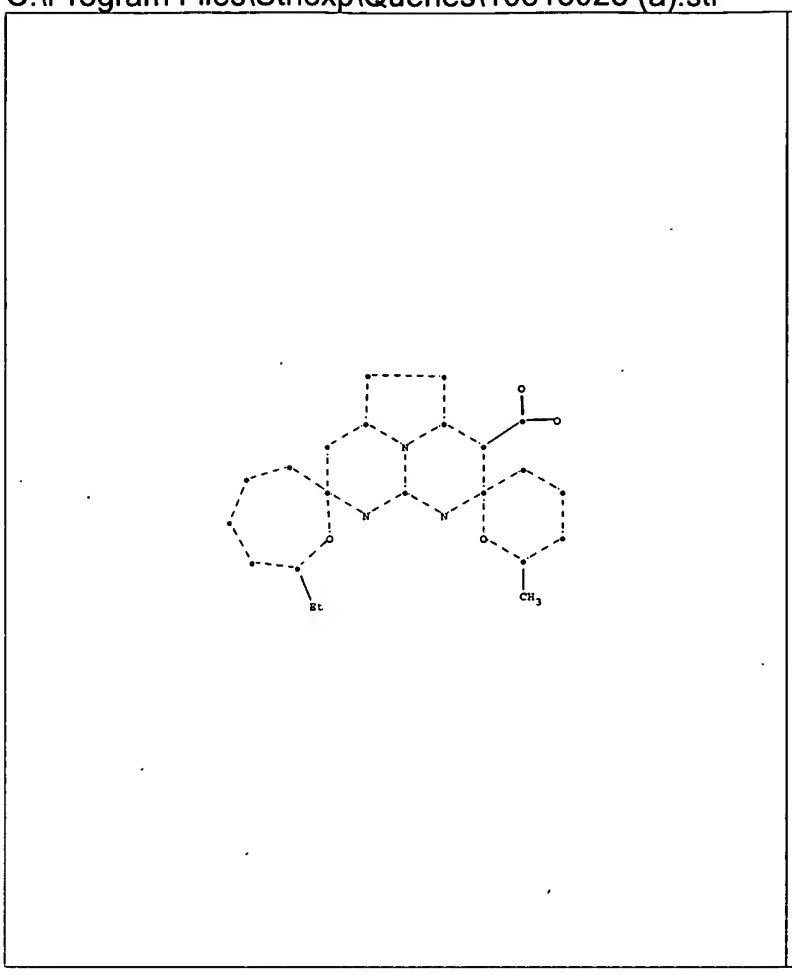
EAST Search History

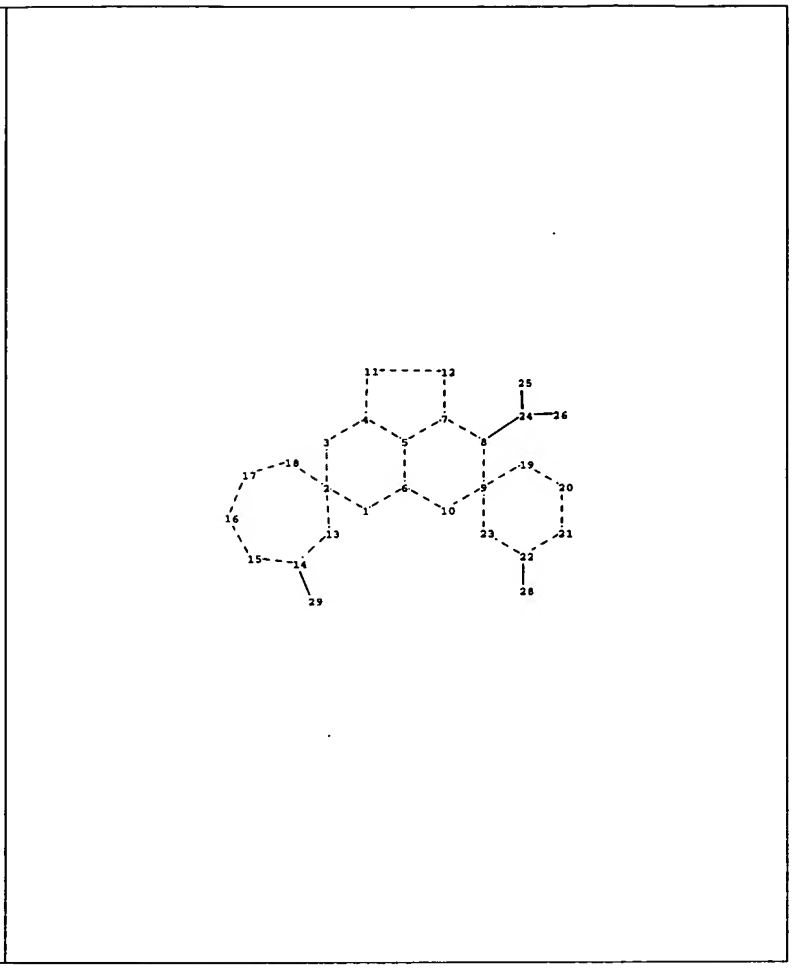
Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	790	((544/231,245) or (514/257)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/09/19 14:17

NPL

		Results
8.	((TITLE-ABSTR-KEY(guanidine alkaloids)) OR (TITLE-ABSTR-KEY(guanidinium alkaloids)) OR (TITLE-ABSTR-KEY(ptilomycalin)) OR (TITLE-ABSTR-KEY (crambescidin))) AND (antifungal or fungal) *[All Sources(- All Sciences -)]*	15
7.	((TITLE-ABSTR-KEY(guanidine alkaloids)) OR (TITLE-ABSTR-KEY(guanidinium alkaloids)) OR (TITLE-ABSTR-KEY(ptilomycalin)) OR (TITLE-ABSTR-KEY (crambescidin))) AND (antitumor or tumor or cancer) *[All Sources(- All Sciences -)]*	18
6.	((TITLE-ABSTR-KEY(guanidine alkaloids)) OR (TITLE-ABSTR-KEY(guanidinium alkaloids)) OR (TITLE-ABSTR-KEY(ptilomycalin)) OR (TITLE-ABSTR-KEY (crambescidin))) AND antiviral *[All Sources(- All Sciences -)]*	11
5.	(TITLE-ABSTR-KEY(guanidine alkaloids)) OR (TITLE-ABSTR-KEY(guanidinium alkaloids)) OR (TITLE-ABSTR-KEY(ptilomycalin)) OR (TITLE-ABSTR-KEY (crambescidin)) *[All Sources(- All Sciences -)]*	63
4.	TITLE-ABSTR-KEY(guanidine alkaloids) *[All Sources(- All Sciences -)]*	38
3.	TITLE-ABSTR-KEY(guanidinium alkaloids) *[All Sources(- All Sciences -)]*	2
2.	TITLE-ABSTR-KEY(ptilomycalin) *[All Sources(- All Sciences -)]*	22
1.	TITLE-ABSTR-KEY(crambescidin) *[All Sources(- All Sciences -)]*	21

C:\Program Files\Stnexp\Queries\10815023 (a).str





chain nodes :
24 25 26 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
8-24 14-29 22-28 24-25 24-26
ring bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10 9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
exact/norm bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10 9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23 24-25 24-26
exact bonds :
8-24 14-29 22-28
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 28:CLASS 29:CLASS

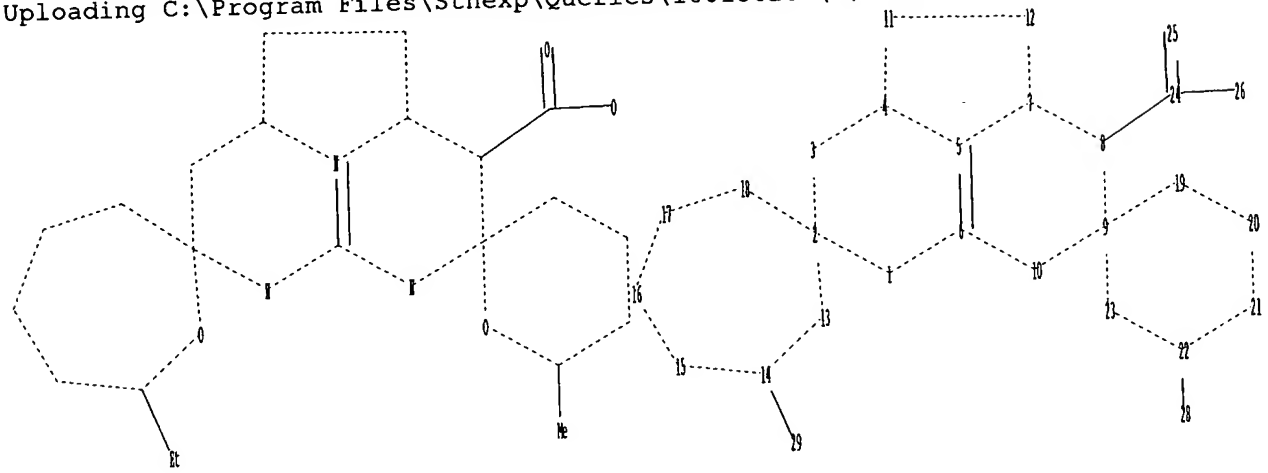
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 964 AND 1006 AND 2040

L1 SCREEN CREATED

=>
Uploading C:\Program Files\Stnexp\Queries\10815023 (b).str

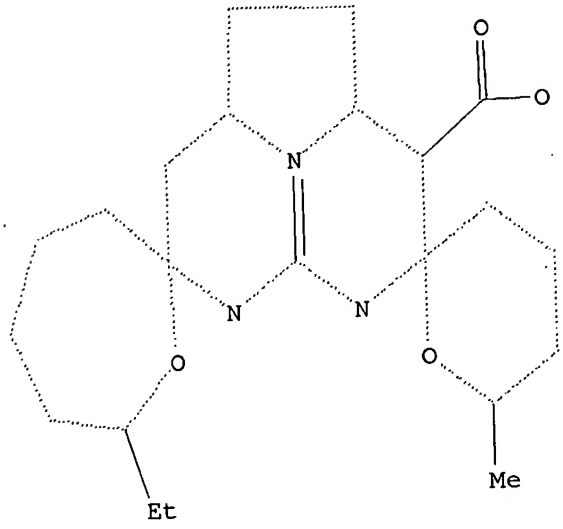


chain nodes :
24 25 26 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
8-24 14-29 22-28 24-25 24-26
ring bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10
9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
exact/norm bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10
9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
24-25 24-26
exact bonds :
8-24 14-29 22-28
isolated ring systems :
containing 1 :

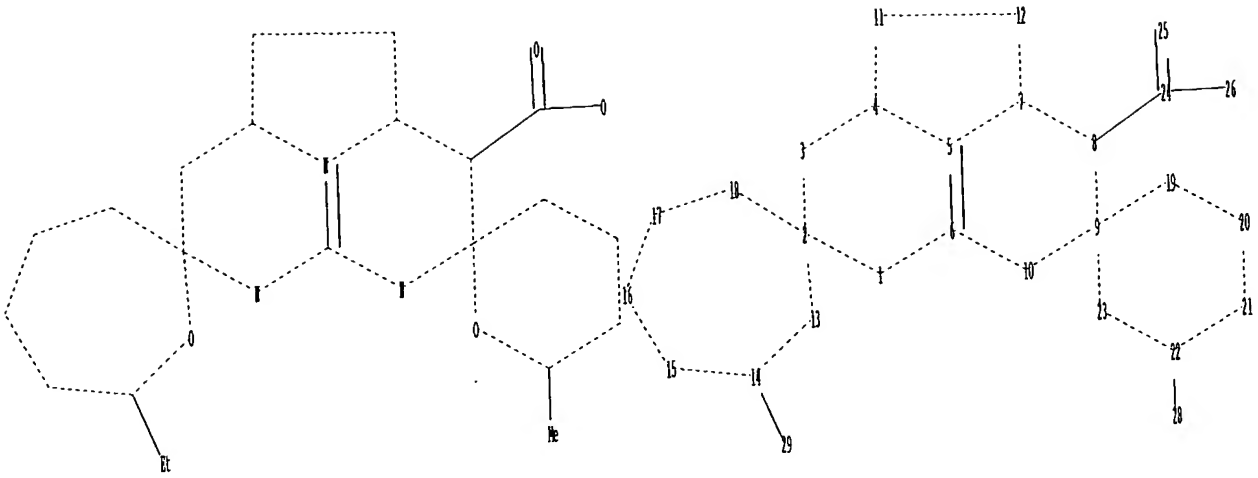
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 28:CLASS
29:CLASS

L2 STRUCTURE UPLOADED

```
=> que L2 AND L1

L3   QUE L2 AND L1

=> d l3
L3 HAS NO ANSWERS
L1              SCR 964 AND 1006 AND 2040
L2              STR
```




```
Structure attributes must be viewed using STN Express query preparation.
L3              QUE  L2 AND L1


=> s l3 sss sam
SAMPLE SEARCH INITIATED 12:45:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        1 TO ITERATE

                                                                0 ANSWERS
100.0% PROCESSED         1 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**

PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               0 TO        0

L4            0 SEA SSS SAM L2 AND L1

=>
Uploading C:\Program Files\Stnexp\Queries\10815023 (c).str
```

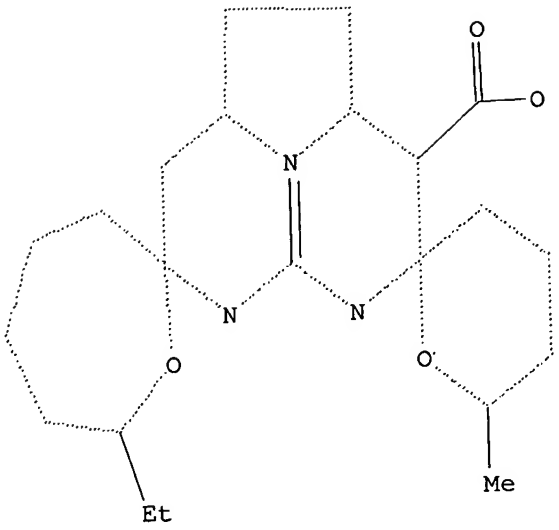


chain nodes :
24 25 26 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
8-24 14-29 22-28 24-25 24-26
ring bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10
9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
exact/norm bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10
9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
24-25 24-26
exact bonds :
8-24 14-29 22-28
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 28:CLASS
29:CLASS

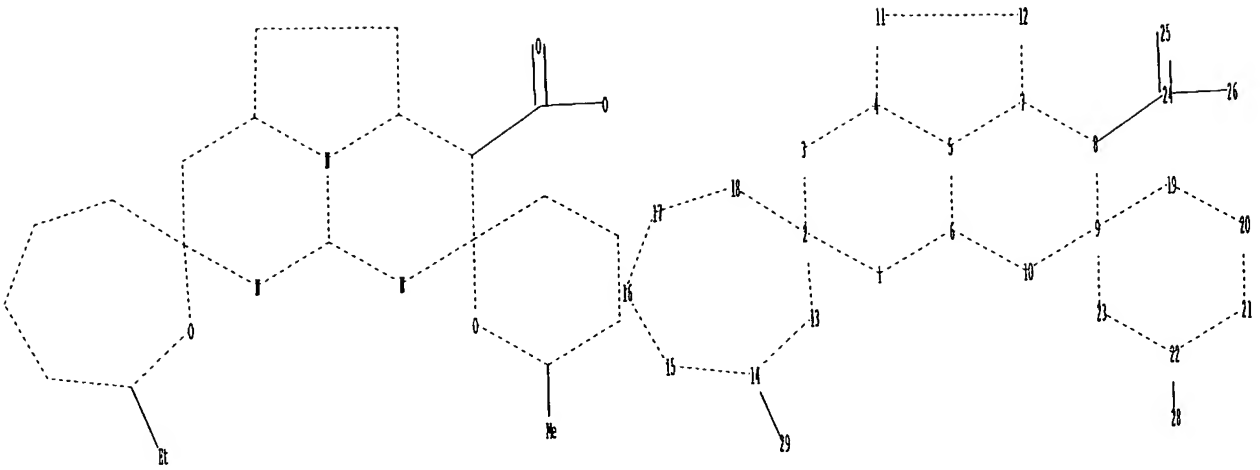
L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l5 sss sam
SAMPLE SEARCH INITIATED 12:47:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       13 TO ITERATE

                                                                0 ANSWERS
100.0% PROCESSED       13 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           44 TO      476
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

=> s l5 sss ful
FULL SEARCH INITIATED 12:47:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      228 TO ITERATE

                                                                0 ANSWERS
100.0% PROCESSED      228 ITERATIONS
SEARCH TIME: 00.00.01

L7            0 SEA SSS FUL L5

=>
Uploading C:\Program Files\Stnexp\Queries\10815023 (a).str
```

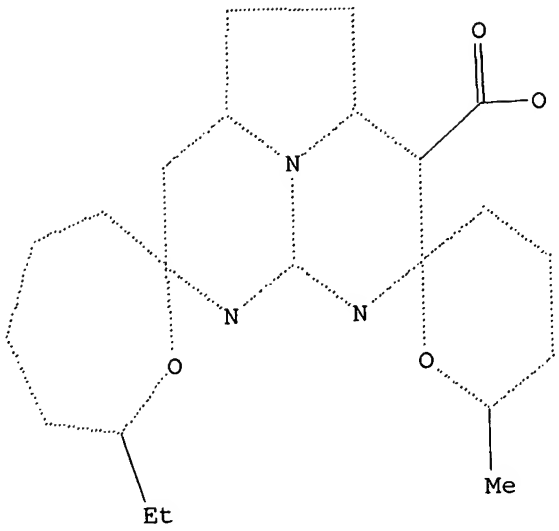


chain nodes :
24 25 26 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
8-24 14-29 22-28 24-25 24-26
ring bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10
9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
exact/norm bonds :
1-2 1-6 2-3 2-13 2-18 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-12 8-9 9-10
9-19 9-23 11-12 13-14 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
24-25 24-26
exact bonds :
8-24 14-29 22-28
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 28:CLASS
29:CLASS

L8 STRUCTURE UPLOADED

=> d l8
L8 HAS NO ANSWERS
L8 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l8 sss sam
SAMPLE SEARCH INITIATED 12:48:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       13 TO ITERATE

                                                                  9 ANSWERS
100.0% PROCESSED       13 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           44 TO      476
PROJECTED ANSWERS:               9 TO      360

L9            9 SEA SSS SAM L8

=> s l8 sss ful
FULL SEARCH INITIATED 12:48:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      228 TO ITERATE

                                                                 176 ANSWERS
100.0% PROCESSED      228 ITERATIONS
SEARCH TIME: 00.00.01

L10          176 SEA SSS FUL L8

=> => s l10
L11          63 L10

=> d l11 1-63 bib,ab,hitstr
```

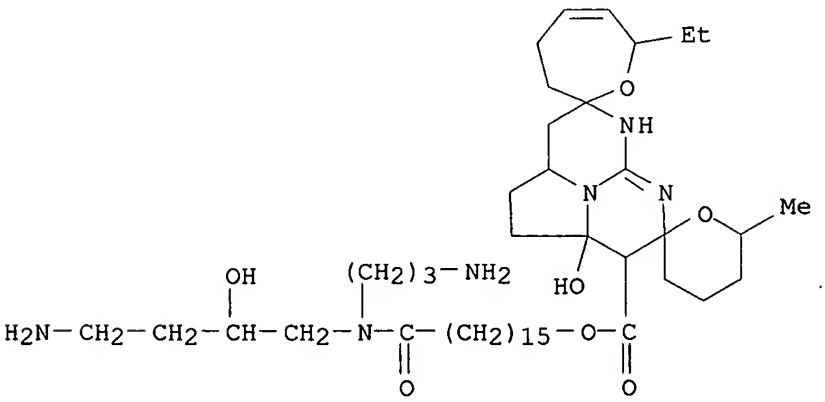
L11 ANSWER 1 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2006:100738 CAPLUS
DN 144:198849
TI Novel dosage form comprising modified-release and immediate-release active ingredients
IN Vaya, Navin; Karan, Rajesh Singh; Sadanand, Sunil; Gupta, Vinod Kumar
PA India
SO U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 630,446.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2006024365	A1	20060202	US 2005-134633	20050519
	IN 193042	A	20040626	IN 2002-MU697	20020805
	US 2004096499	A1	20040520	US 2003-630446	20030729
PRAI	IN 2002-MU697	A	20020805		
	IN 2002-MU699	A	20020805		
	IN 2003-MU80	A	20030122		
	IN 2003-MU82	A	20030122		
	US 2003-630446	A2	20030729		

AB A dosage form comprising of a high dose, high solubility active ingredient as modified release and a low dose active ingredient as immediate release where the weight ratio of immediate release active ingredient and modified release active ingredient is from 1:10 to 1:15000 and the weight of modified release active ingredient per unit is from 500 mg to 1500 mg; a process for preparing the dosage form. Tablets containing 10 mg sodium pravastatin and 1000 mg niacin were prepared The release of sodium pravastatin after 24 h was 67.7%, and the release of niacin after 1 h was 84.1%.

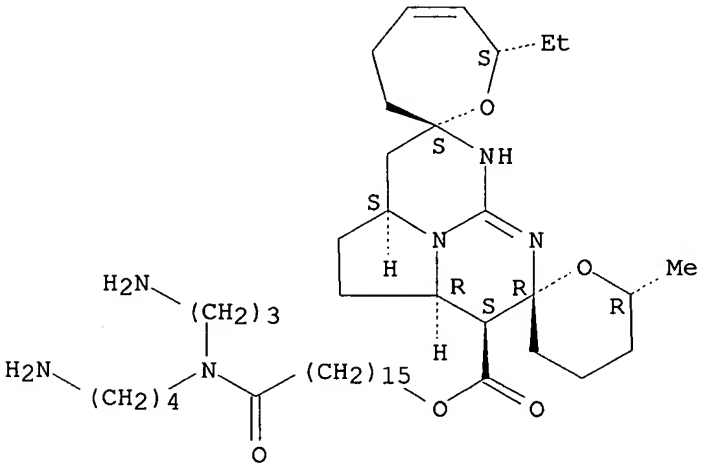
IT 135257-45-3, Crambescidin 816
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)

RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



L11 ANSWER 2 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:821020 CAPLUS
DN 143:363656
TI Alkaloids from the sponge Monanchora unguifera
AU Gallimore, Winklet A.; Kelly, Michelle; Scheuer, Paul J.
CS Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI, 96822, USA
SO Journal of Natural Products (2005), 68(9), 1420-1423
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society-American Society of Pharmacognosy
DT Journal
LA English
AB The bioassay-guided fractionation of the cytotoxic crude gum obtained from the Caribbean sponge Monanchora unguifera led to the isolation and characterization of the new compds. batzelladine J (I) and crambescidic acid (II) in addition to known guanidine alkaloids ptilomycalin A, ptilocaulin, and isoptilocaulin. The structures of the compds. were elucidated by interpretation of the 1D and 2D NMR expts. The chemotaxonomic implications of these findings are discussed.
IT 124512-47-6, Ptilomycalin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(alkaloids from sponge Monanchora unguifera)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

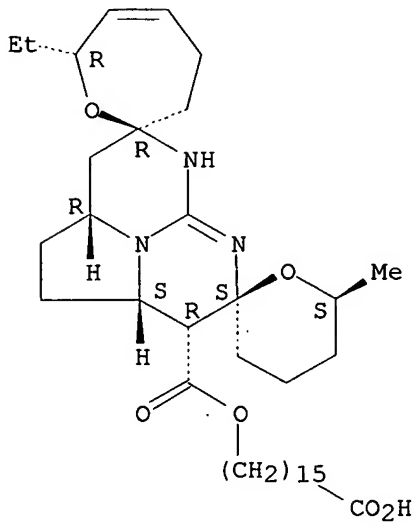
Absolute stereochemistry. Rotation (-).



IT 866403-34-1P, Crambescidic acid
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(alkaloids from sponge Monanchora unguifera)
RN 866403-34-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester,

(2R,2''S,2'aR,6''S,7R,8'R,8'aS)-rel-(+)- (9CI) (CA INDEX NAME)

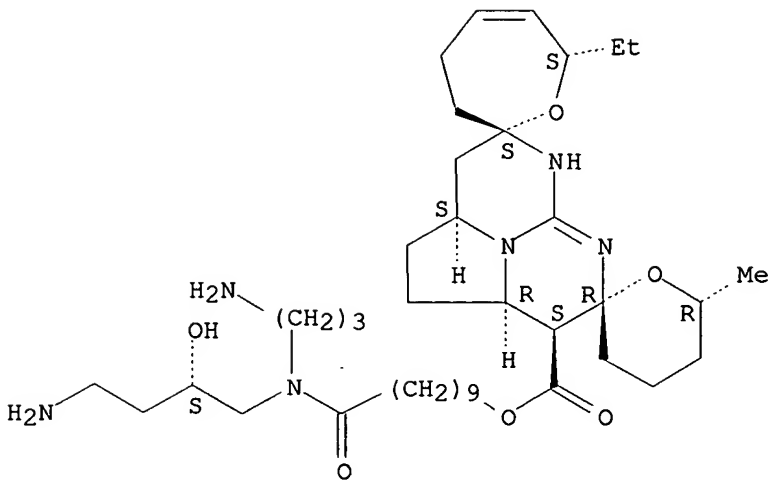
Rotation (+). Absolute stereochemistry unknown.
Currently available stereo shown.



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:777878 CAPLUS
DN 143:339016
TI Library versus library recognition and inhibition of the HIV-1 Nef allelome
AU Olszewski, Allison; Weiss, Gregory A.
CS Departments of Chemistry, Molecular Biology and Biochemistry, University of California, Irvine, CA, 92697-2025, USA
SO Journal of the American Chemical Society (2005), 127(35), 12178-12179
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Rapid evolution of drug-resistant viruses renders essentially all small-mol. antiviral treatments ineffective. The authors demonstrate an in vitro library vs. library approach to identify small mols. targeting a broad spectrum of HIV-1 Nef protein variants. The technique could provide more effective antiviral therapies. First, a library of clin. derived Nef allelic variants, termed an allelome, was selected for function by binding to Nef ligands p53, actin, or p56lck. Next, a library of small-mol. inhibitors challenged the Nef allelome in competition assays. In contrast to single-variant inhibition, structurally simpler mols. could better inhibit the Nef allelome. Addnl., Nef sequences selected for binding to p53 resembled sequences from patients with a rapid progression to AIDS phenotype. Thus, the allelome vs. small-mol. library approach offers a route for improving antiviral drug discovery and elucidating fundamental mechanisms of viral pathogenesis and resistance.
IT 600706-88-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(library vs. library recognition and inhibition of HIV-1 Nef allelome)
RN 600706-88-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-10-oxodecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●3 HCl

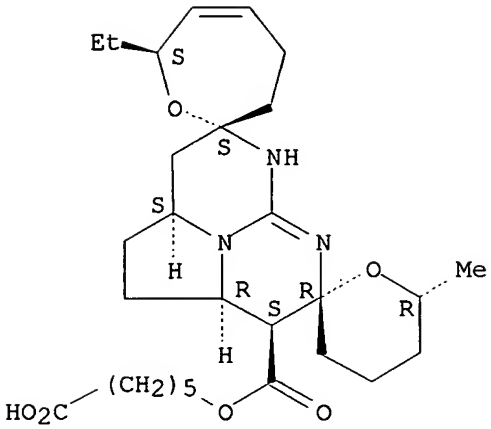
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:139449 CAPLUS
DN 142:392557
TI Total Synthesis and Properties of the Crambescidin Core Zwitterionic Acid and Crambescidin 359
AU Aron, Zachary D.; Overman, Larry E.
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Journal of the American Chemical Society (2005), 127(10), 3380-3390
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 142:392557
AB The total synthesis of the crambescidin core acid (I; R = CO2-), crambescidins 359 (I; R = H, X = Cl-) and 431 (I; R = CO2Et, X = CF2CO2-), and the properties of the crambescidin core are described. A key step of the synthetic route to guanidinium carboxylate I (R = CO2-) is Pd(0) catalyzed cleavage of the ester side chain of pentacyclic cinnamyl ester I [R = CO2CH2CH:CHPh-(E), X = HCO2-]. This ester is also employed to prepare a small library of crambescidin alkaloid analogs that differ in their C14 side chain. The zwitterionic guanidinium carboxylate I (R = CO2-) was shown to readily decarboxylate to form crambescidin 359 (I; R = H, X = Cl-). Decarboxylation of crambescidin core acid I (R = CO2-) was fastest under basic conditions. In the presence of base, up to eight deuterium atoms can be incorporated into the pentacyclic crambescidin core. Both deuterium incorporation and decarboxylation of crambescidin core acid I (R = CO2-) are the result of facile ring opening of the spirocyclic ether rings of the pentacyclic guanidinium moiety.
IT 849724-20-5DP, zwitterionic tautomer 849724-23-8DP, zwitterionic tautomer 849724-28-3DP, zwitterionic tautomer 849724-30-7DP, zwitterionic tautomer 849724-33-0DP, zwitterionic tautomer 849724-36-3DP, zwitterionic tautomer
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, by hydroxyspermidine derivative; total synthesis
and properties of the crambescidin core zwitterionic acid and crambescidin 359)
RN 849724-20-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 5-carboxypentyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

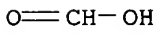
CRN 600706-81-8
CMF C28 H43 N3 O6

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

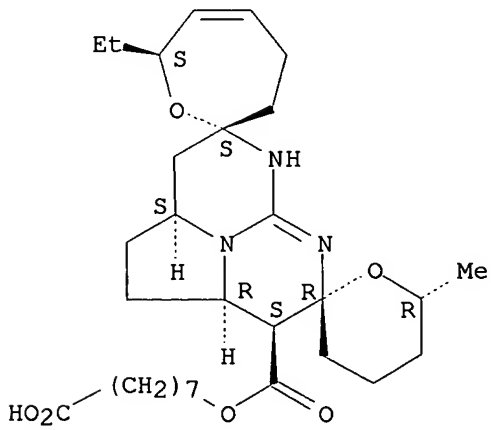


RN 849724-23-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 7-carboxyheptyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 600706-93-2
CMF C30 H47 N3 O6

Absolute stereochemistry.



CM 2

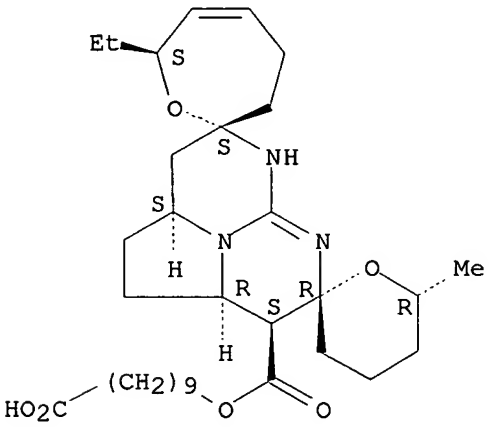
CRN 64-18-6
CMF C H2 O2

RN 849724-28-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 9-carboxynonyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

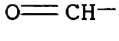
CRN 600706-98-7
CMF C32 H51 N3 O6

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

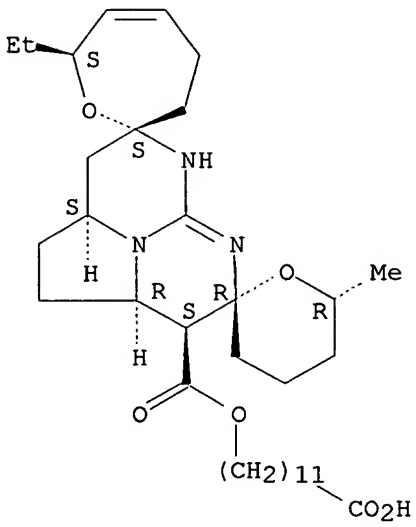


RN 849724-30-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 11-carboxyundecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

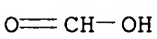
CRN 600706-99-8
CMF C34 H55 N3 O6

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

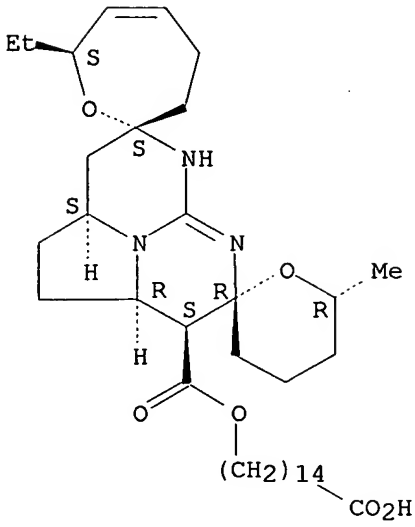


RN 849724-33-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 14-carboxytetradecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

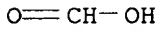
CRN 600707-00-4
CMF C37 H61 N3 O6

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

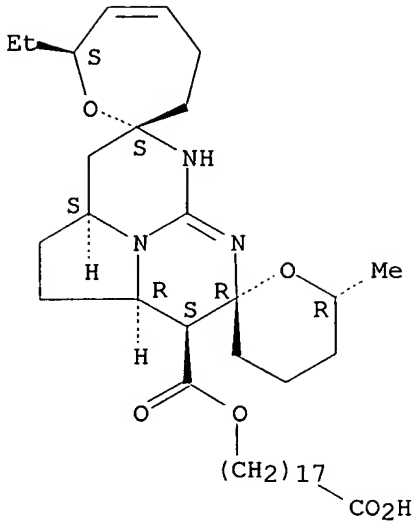


RN 849724-36-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 17-carboxyheptadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

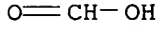
CRN 600707-01-5
CMF C40 H67 N3 O6

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2



IT 849724-25-0DP, zwitterionic tautomer 849724-27-2DP, zwitterionic tautomer 849724-29-4DP, zwitterionic tautomer 849724-32-9DP, zwitterionic tautomer 849724-35-2DP, zwitterionic tautomer 849724-37-4DP, zwitterionic tautomer
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of; total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

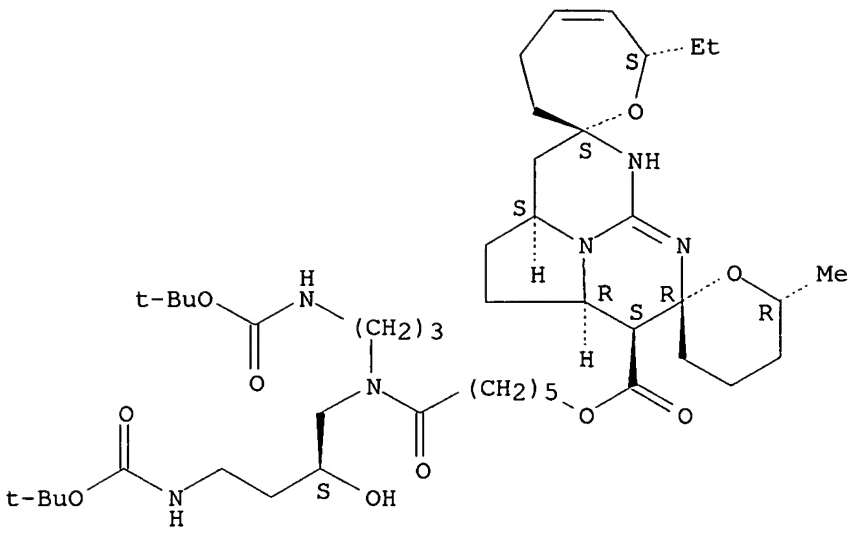
RN 849724-25-0 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-6-oxohexyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

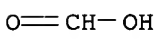
CRN 791583-90-9
CMF C45 H76 N6 O10

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

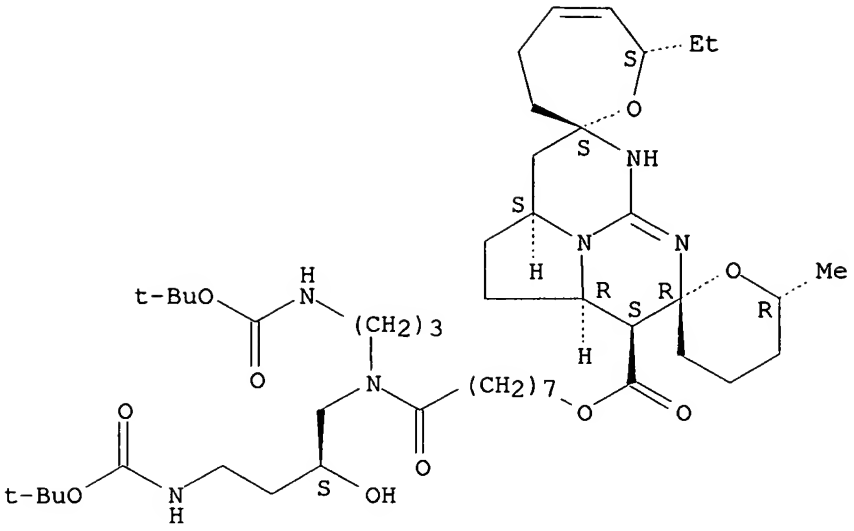


RN 849724-27-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 8-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-8-oxooctyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

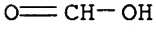
CRN 785774-22-3
CMF C47 H80 N6 O10

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

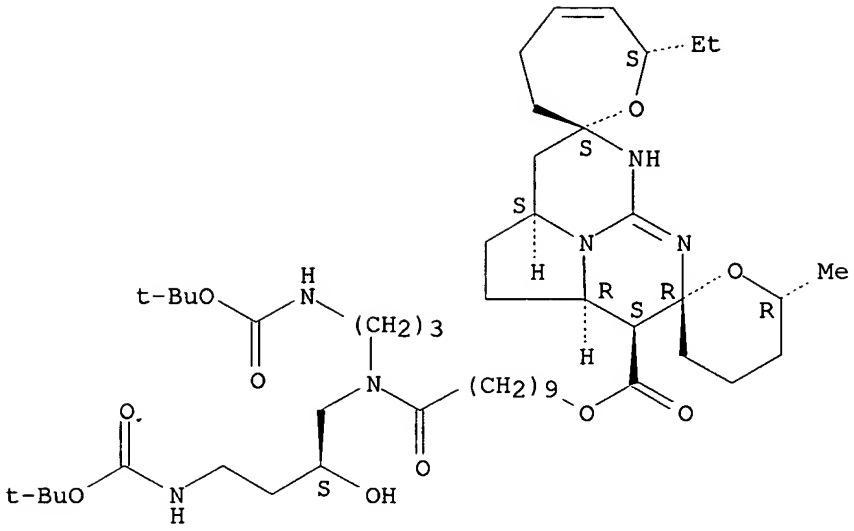


RN 849724-29-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-10-oxodecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 746603-55-4
CMF C49 H84 N6 O10

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

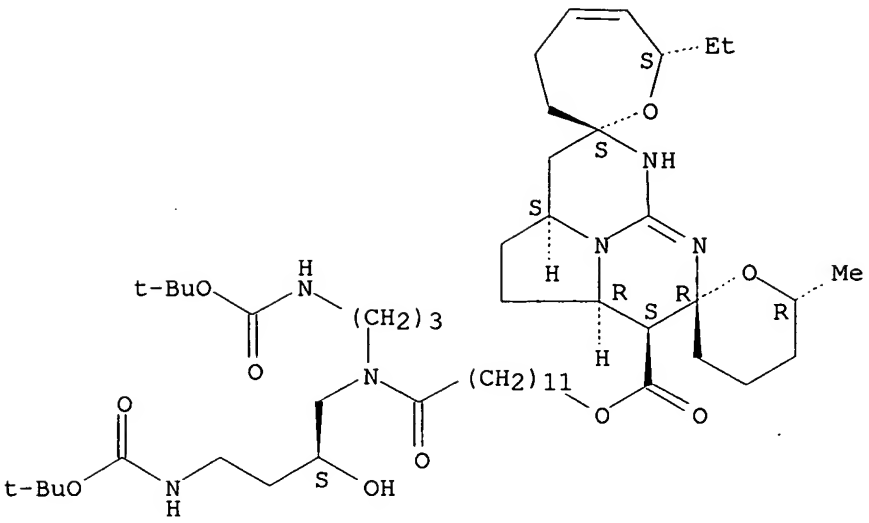
O═CH—OH

RN 849724-32-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 12-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-12-oxododecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 765268-38-0
CMF C51 H88 N6 O10

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

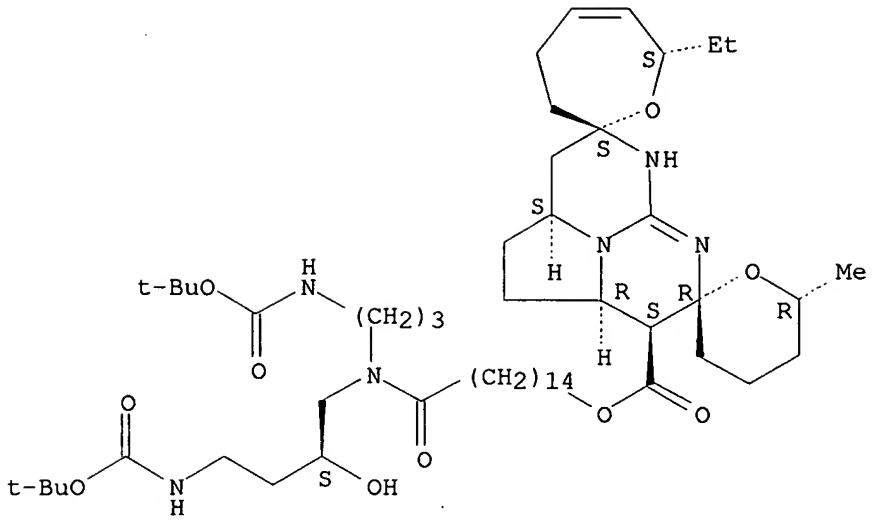
O═CH—OH

RN 849724-35-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-15-oxopentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 754975-46-7
CMF C54 H94 N6 O10

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

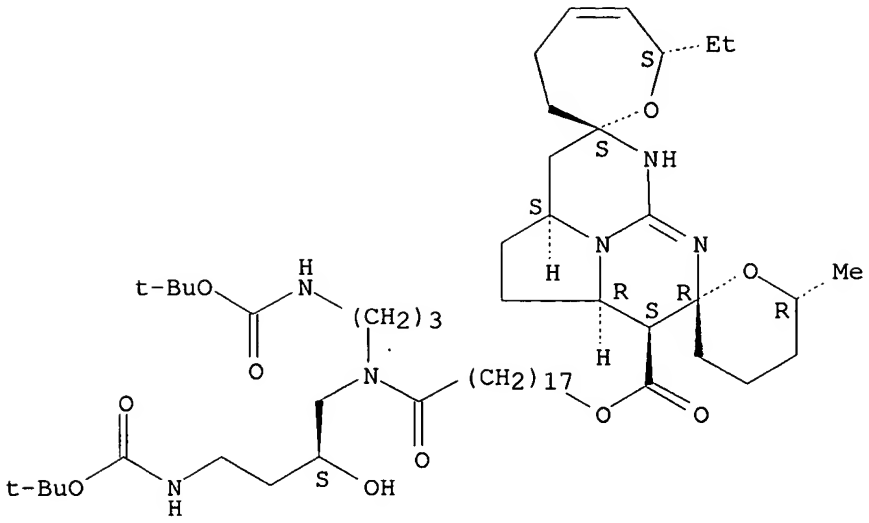
O═CH—OH

RN 849724-37-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-18-oxooctadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 783302-30-7
CMF C57 H100 N6 O10

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

O═CH—OH

IT 849724-17-0DP, zwitterionic tautomer
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and epimerization of; total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

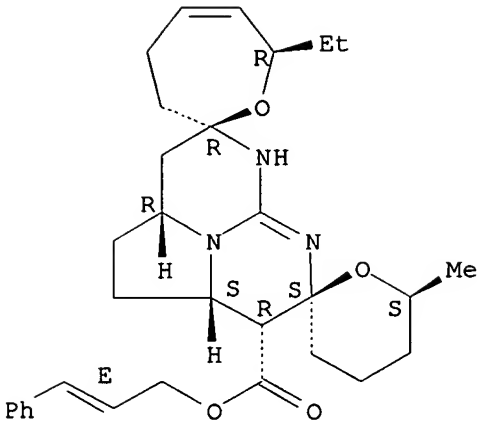
RN 849724-17-0 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2R,2''S,2'aR,6''S,7R,8'R,8'aS)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 849724-16-9
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



CM 2

CRN 64-18-6
CMF C H2 O2

O═CH—OH

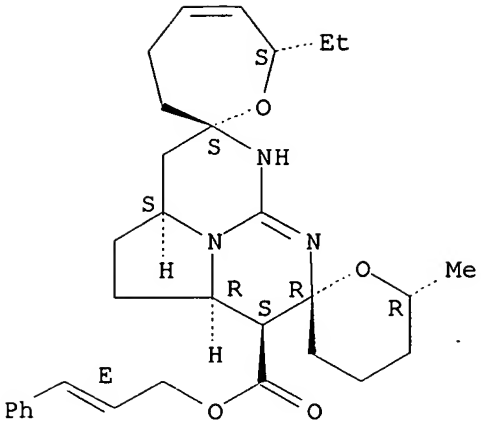
IT 600707-02-6DP, zwitterionic tautomer
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and palladium-catalyzed de-esterification of; total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

RN 600707-02-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 600706-77-2
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



CM 2

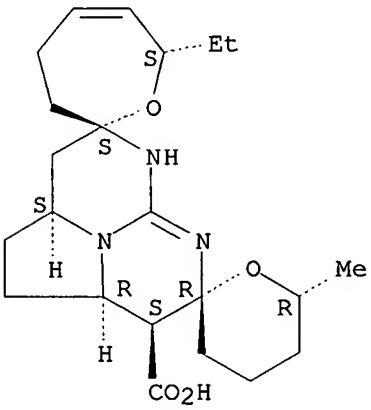
CRN 64-18-6
CMF C H2 O2

IT 147664-30-0DP, Crambescidin core acid, zwitterionic tautomer
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure and decarboxylation of; total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

RN 147664-30-0 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

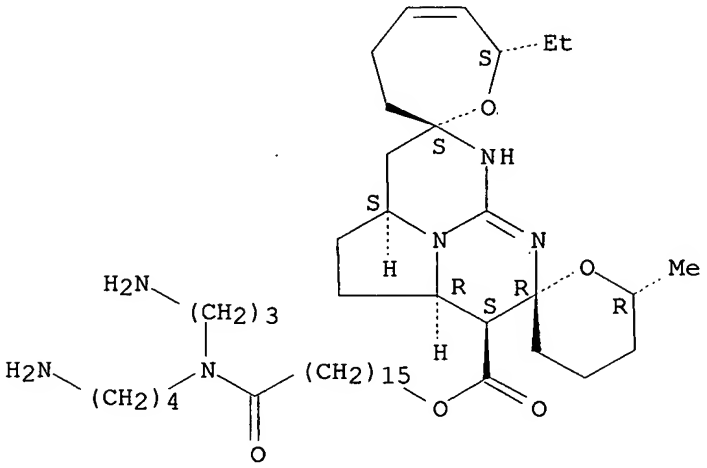


IT 124512-47-6P, Ptilomycalin A 135257-45-3P, Crambescidin 816 135257-46-4P, Crambescidin 800 135257-47-5P, Crambescidin 830 135283-73-7P, Crambescidin 844 163597-72-6P, Celeromycalin 214215-58-4P, Crambescidin 657 229160-50-3P, Neofolitispate 1 229160-51-4P, Neofolitispate 2 229160-52-5P, Neofolitispate 3
RL: PNU (Preparation, unclassified); PREP (Preparation)
(total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

RN 124512-47-6 CAPLUS

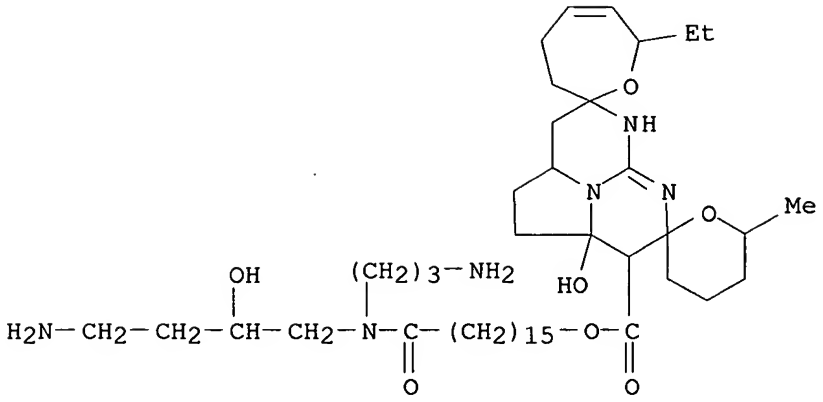
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



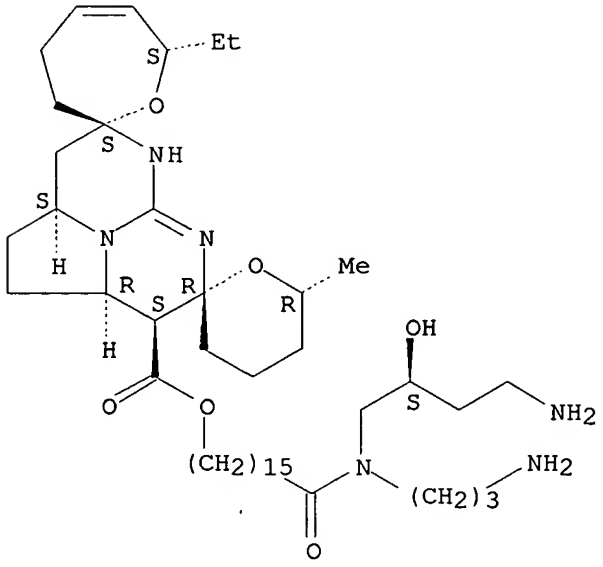
RN 135257-45-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

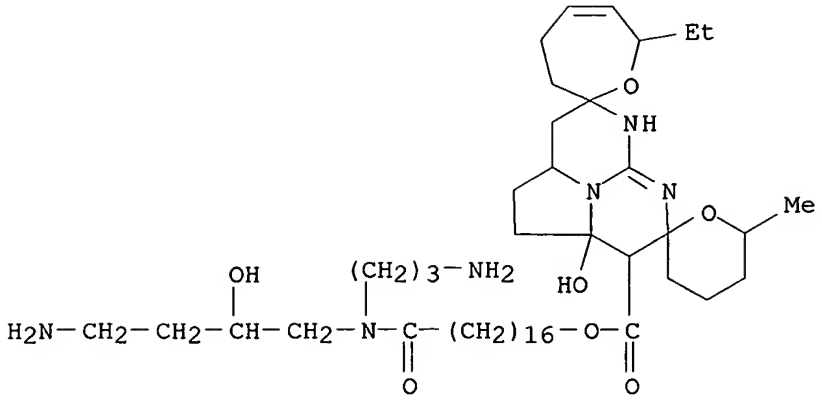


RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

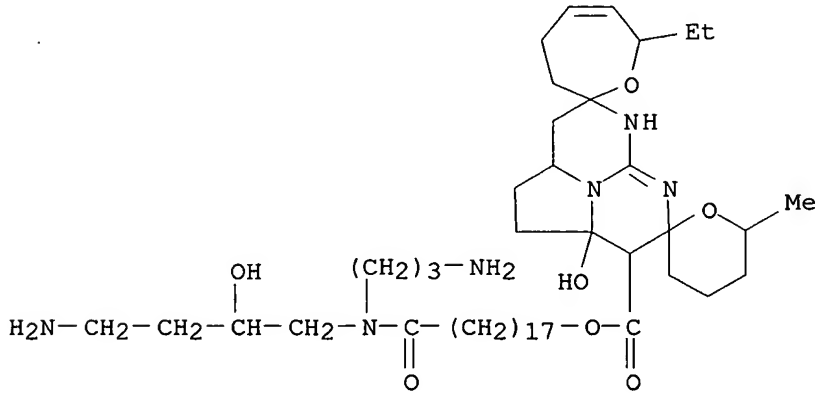
Absolute stereochemistry. Rotation (-).



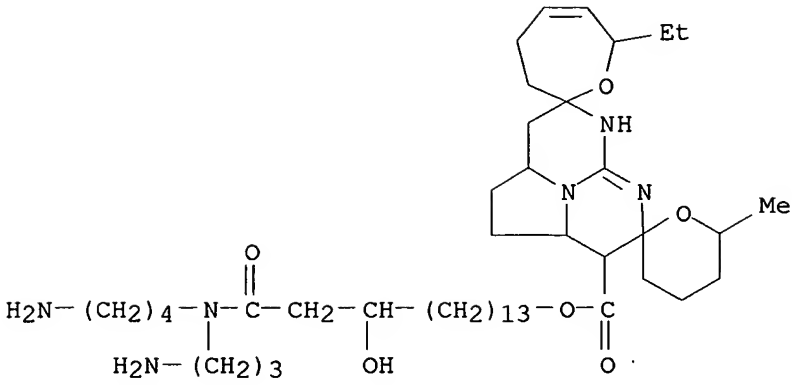
RN 135257-47-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 17-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-17-oxoheptadecyl ester (9CI) (CA INDEX NAME)



RN 135283-73-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 18-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-18-oxooctadecyl ester (9CI) (CA INDEX NAME)

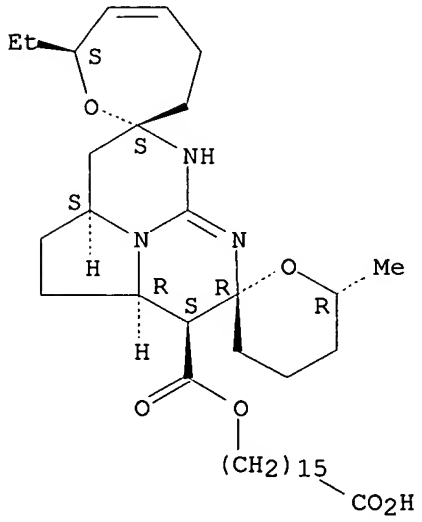


RN 163597-72-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (14R)-16-[(4-aminobutyl)(3-aminopropyl)amino]-14-hydroxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)



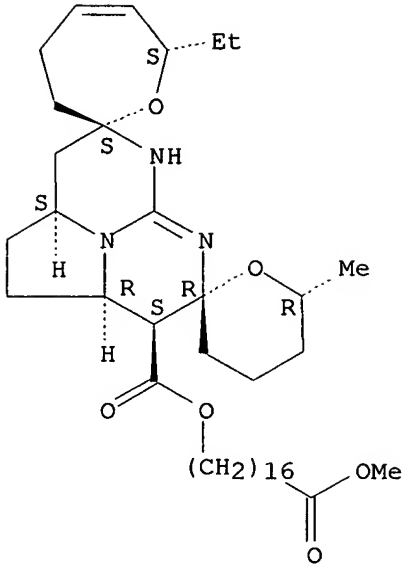
RN 214215-58-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



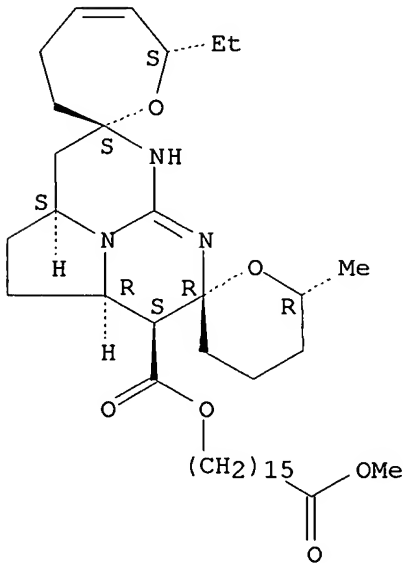
RN 229160-50-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 17-methoxy-17-oxoheptadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



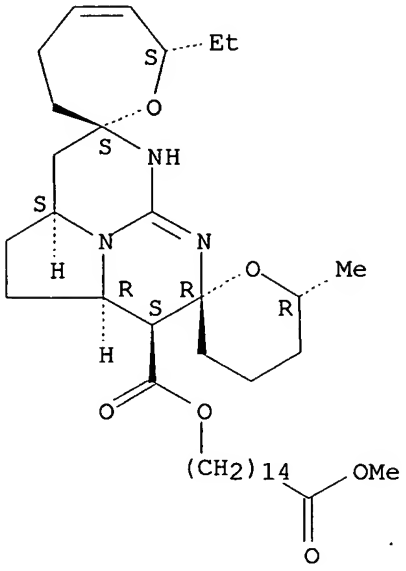
RN 229160-51-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-methoxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 229160-52-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-methoxy-15-oxopentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 600706-78-3DP, zwitterionic tautomer
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

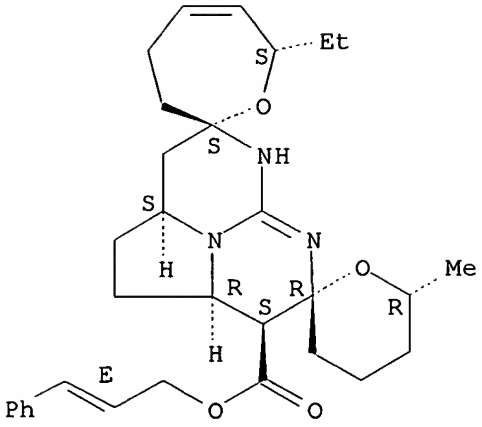
RN 600706-78-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

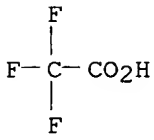
CRN 600706-77-2
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



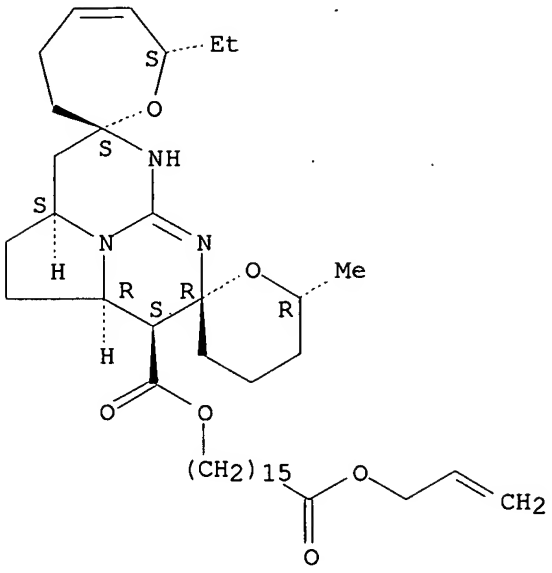
IT 162145-90-6DP, zwitterionic tautomer 259734-00-4P, Crambescidin 431 316831-29-5DP, zwitterionic tautomer 600706-83-0DP, zwitterionic tautomer 600706-87-4DP, zwitterionic tautomer 600706-88-5DP, zwitterionic tautomer 600706-89-6DP, zwitterionic tautomer 600706-90-9DP, zwitterionic tautomer 600706-91-0DP, zwitterionic tautomer 732299-90-0DP, zwitterionic tautomer 732299-92-2DP, zwitterionic tautomer 849724-19-2DP, zwitterionic tautomer 849724-22-7DP, zwitterionic tautomer 849724-24-9DP, zwitterionic tautomer 849927-04-4DP, Crambescidin 431 trifluoroacetate, zwitterionic tautomer 849927-06-6DP, Crambescidin acid core trifluoroacetate, zwitterionic tautomer
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis and properties of the crambescidin core zwitterionic acid and crambescidin 359)

RN 162145-90-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 162145-89-3
CMF C41 H67 N3 O6

Absolute stereochemistry. Rotation (-).

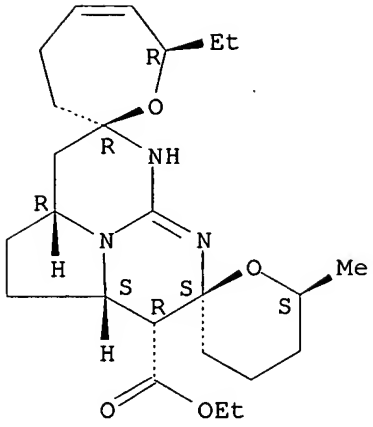


CM 2

CRN 64-18-6
CMF C H2 O2

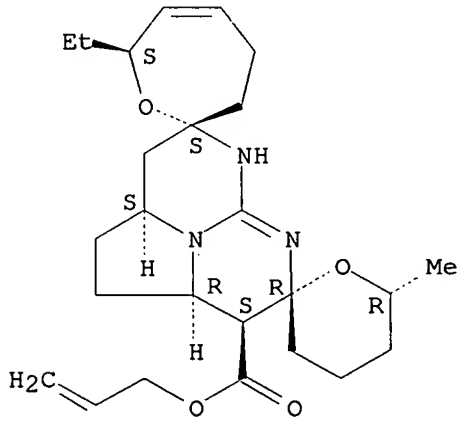
RN 259734-00-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, ethyl ester, (2R,2''S,2'aR,6''S,7R,8'R,8'aS)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.
Currently available stereo shown.



RN 316831-29-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 2-propenyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

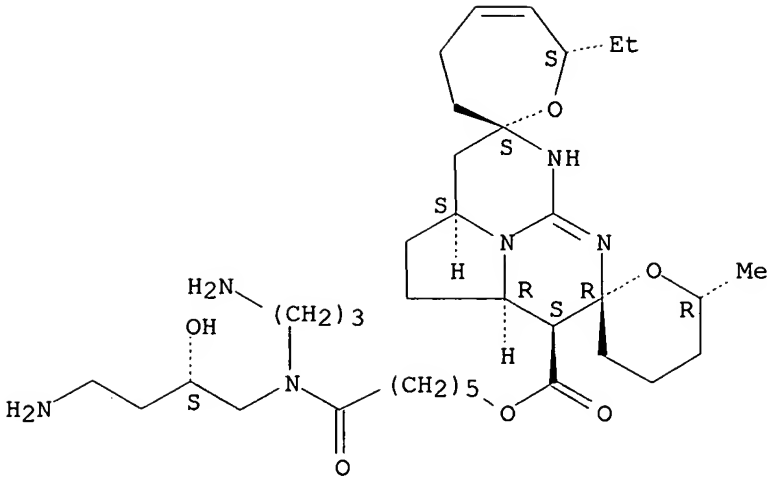
Absolute stereochemistry.



● HCl

RN 600706-83-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-6-oxohexyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

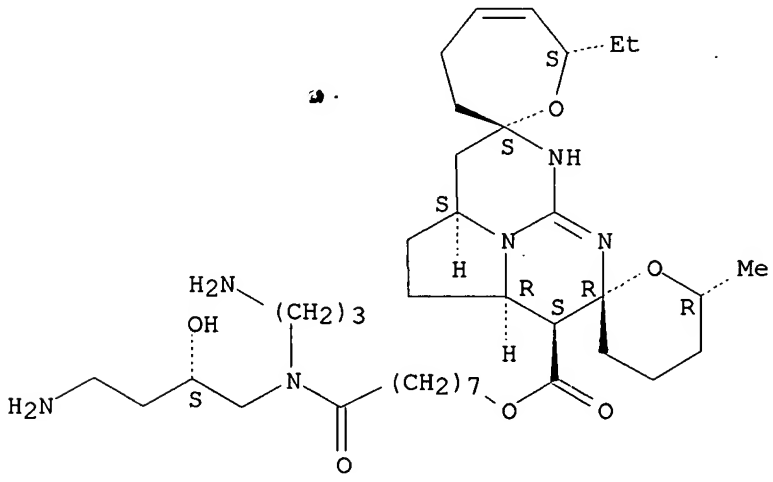
Absolute stereochemistry.



●3 HCl

RN 600706-87-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 8-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-8-oxooctyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

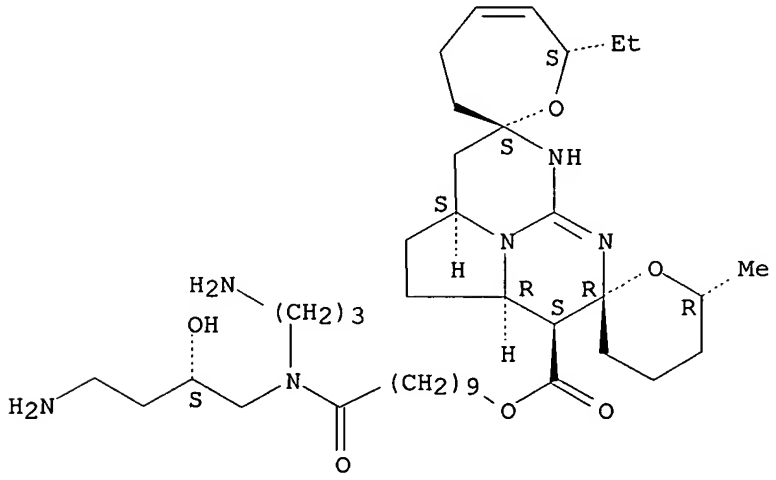


●3 HCl

RN 600706-88-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-10-oxodecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

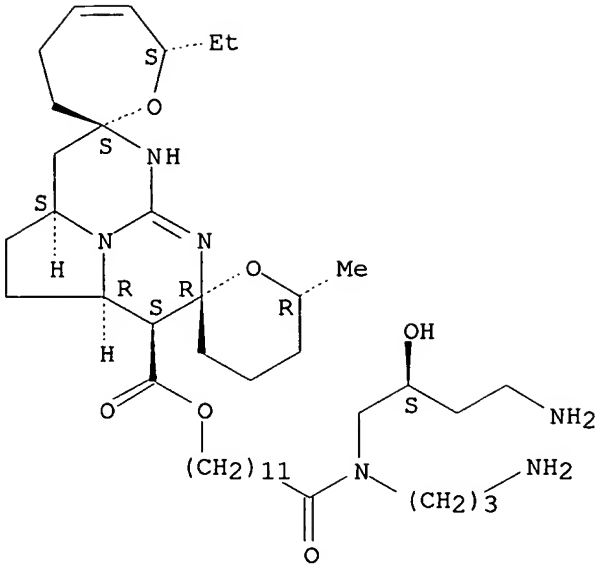


●3 HCl

RN 600706-89-6 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 12-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-12-oxododecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

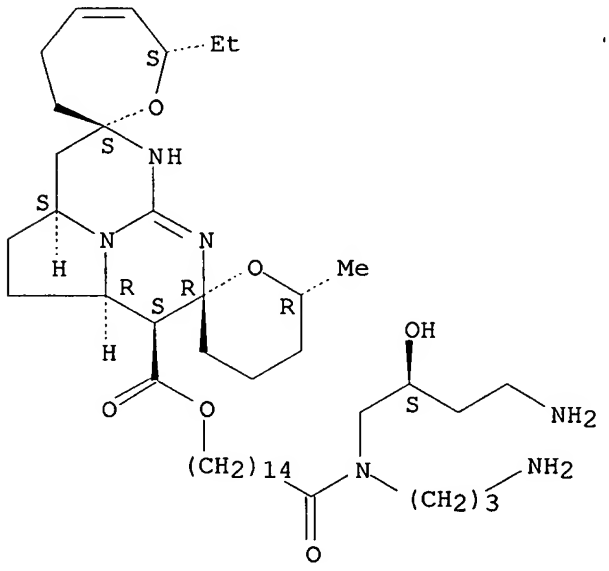
Absolute stereochemistry.



●3 HCl

RN 600706-90-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-15-oxopentadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

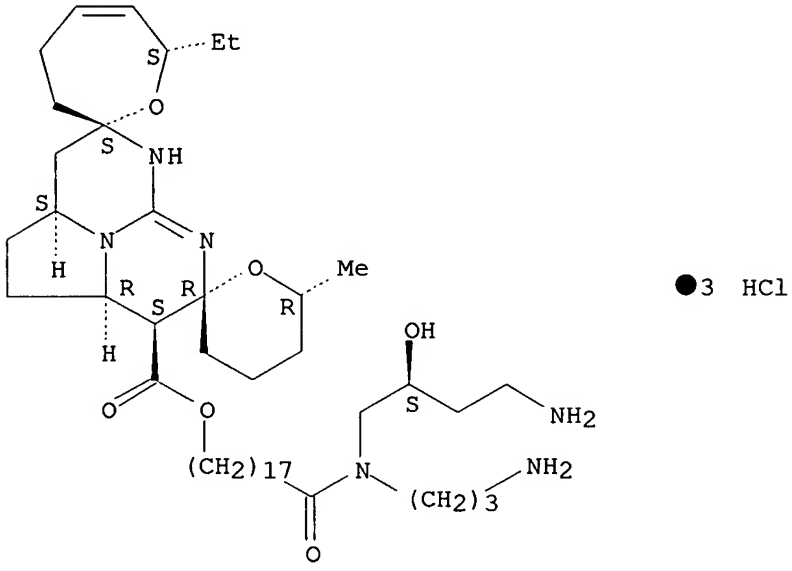


●3 HCl

RN 600706-91-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[[(2S)-4-amino-2-hydroxybutyl](3-

aminopropyl)amino]-18-oxooctadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

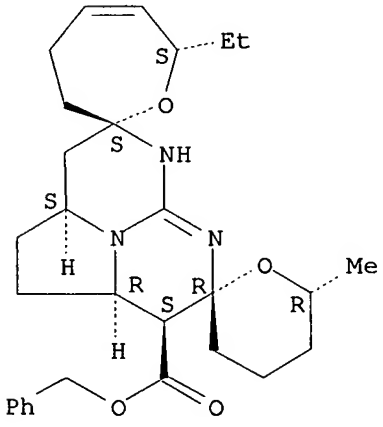


● 3 HCl

RN 732299-90-0 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, phenylmethyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



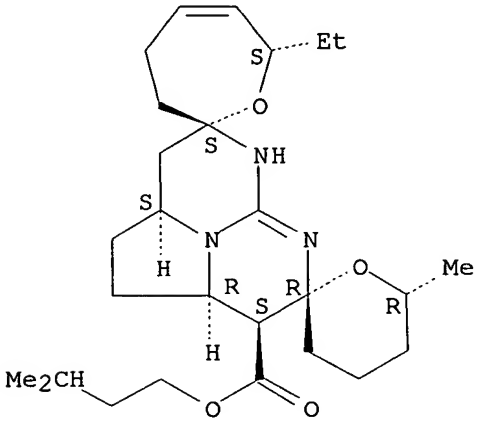
● HCl

RN 732299-92-2 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 3-methylbutyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

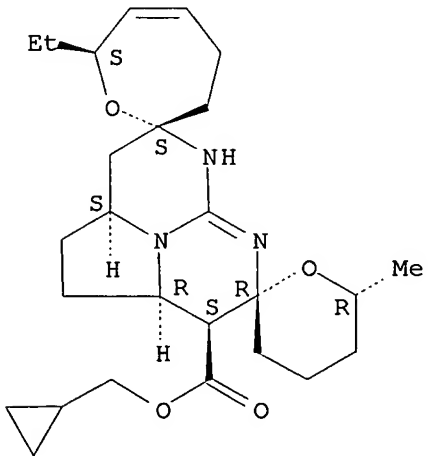


● HCl

RN 849724-19-2 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, cyclopropylmethyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

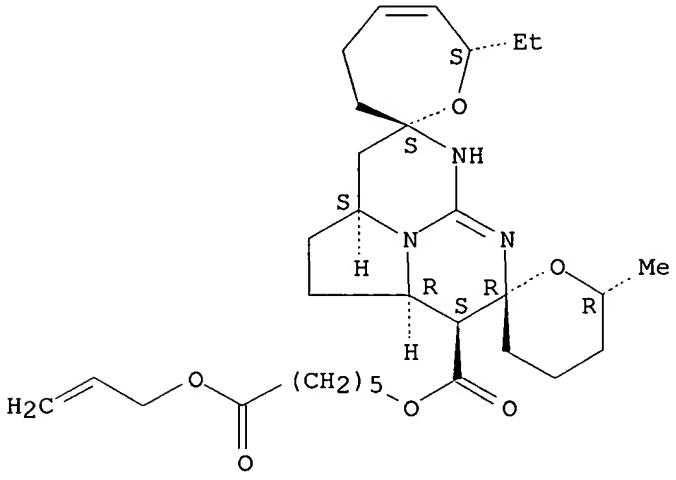
RN 849724-22-7 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-oxo-6-(2-propenyloxy)hexyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 849724-21-6
CMF C31 H47 N3 O6

Absolute stereochemistry.



CM 2

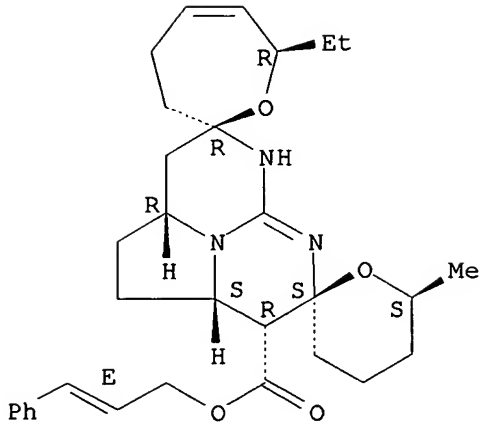
CRN 64-18-6
CMF C H2 O2

RN 849724-24-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2R,2''S,2'aR,6''S,7R,8'R,8'aS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

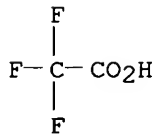
CRN 849724-16-9
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

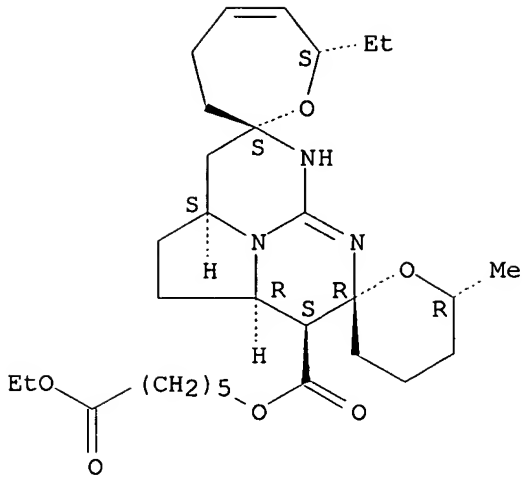


RN 849927-04-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-ethoxy-6-oxohexyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

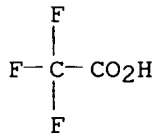
CRN 849927-03-3
CMF C30 H47 N3 O6

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

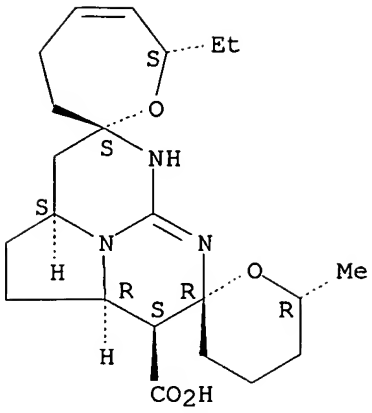


RN 849927-06-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

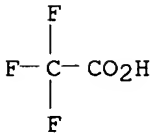
CRN 147664-30-0
CMF C22 H33 N3 O4

Absolute stereochemistry.



CM 2

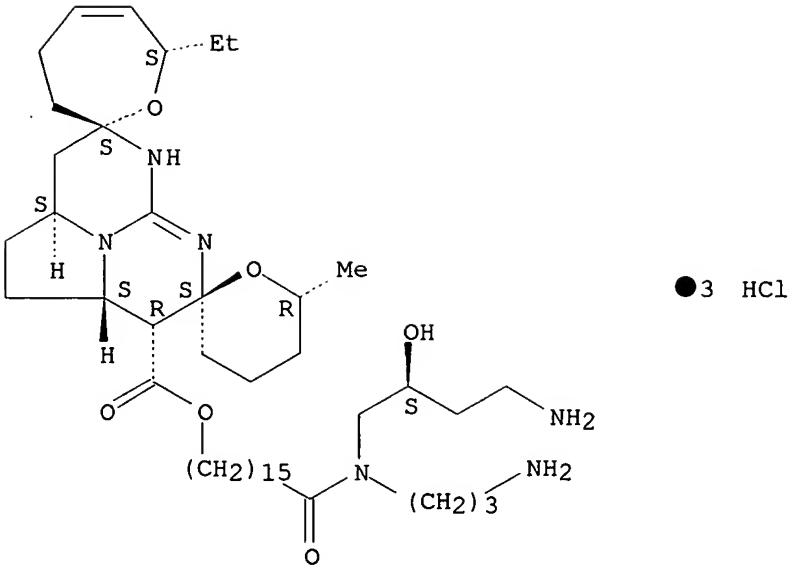
CRN 76-05-1
CMF C2 H F3 O2



RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:848616 CAPLUS
DN 142:16274
TI Guanidine alkaloid analogs as inhibitors of HIV-1 Nef interactions with p53, actin, and p56lck
AU Olszewski, Allison; Sato, Ken; Aron, Zachary D.; Cohen, Frederick; Harris, Aleishia; McDougall, Brenda R.; Robinson, W. Edward, Jr.; Overman, Larry E.; Weiss, Gregory A.
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Proceedings of the National Academy of Sciences of the United States of America (2004), 101(39), 14079-14084
CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
AB With current anti-HIV treatments targeting only 4 of the 15 HIV proteins, many potential viral vulnerabilities remain unexploited. We report small-mol. inhibitors of the HIV-1 protein Nef. In addition to expanding the anti-HIV arsenal, small-mol. inhibitors against untargeted HIV proteins could be used to dissect key events in the HIV lifecycle. Numerous incompletely characterized interactions between Nef and cellular ligands, for example, present a challenge to understanding mol. events during HIV progression to AIDS. Assays with phage-displayed Nef from HIVNL4-3 were used to identify a series of guanidine alkaloid-based inhibitors of Nef interactions with p53, actin, and p56lck. The guanidines, synthetic analogs of batzellidine and crambescidin natural products, inhibit the Nef-ligand interactions with IC50 values in the low micromolar range. In addition, sensitive in vivo assays for Nef inhibition are reported. Although compds. that are effective in vitro proved to be too cytotoxic for cellular assays, the reported Nef inhibitors provide proof-of-concept for disrupting a new HIV target and offer useful leads for drug development.
IT 246851-97-8 275808-01-0 600706-83-0
600706-88-5 732299-90-0 799812-00-3
RL: PAC (Pharmacological activity); BIOL (Biological study)
(guanidine alkaloid analogs as inhibitors of HIV-1 Nef interactions with p53, actin, and p56lck)
RN 246851-97-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

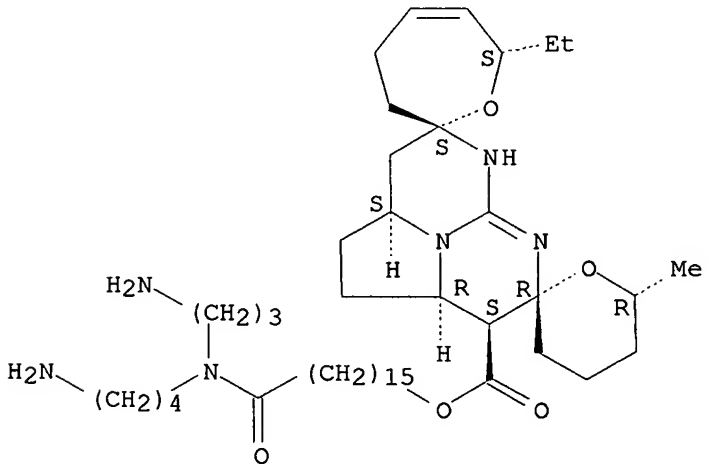
Absolute stereochemistry. Rotation (-).



●3 HCl

RN 275808-01-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

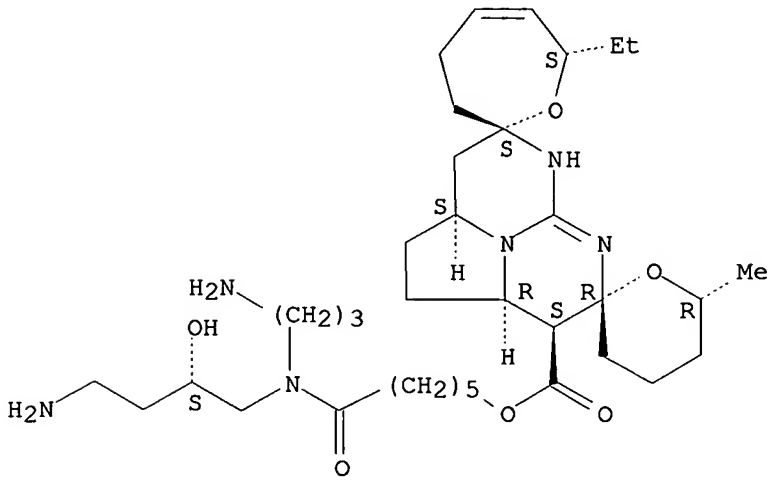


●3 HCl

RN 600706-83-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-amino-2-hydroxybutyl](3-

aminopropyl)amino]-6-oxohexyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

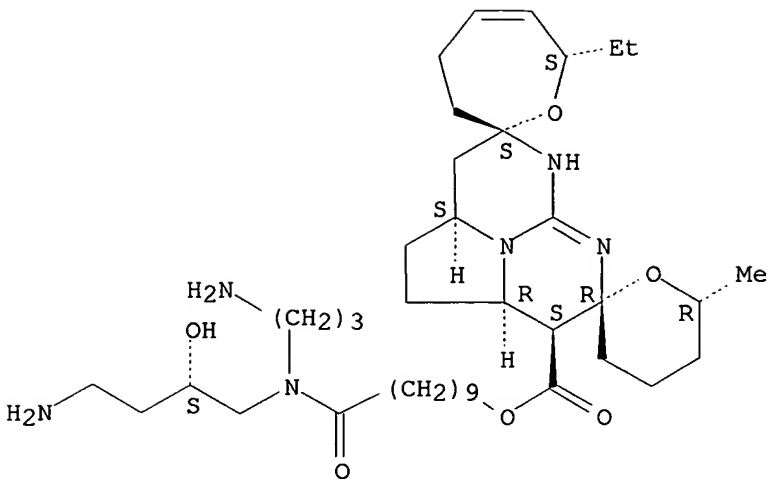


●3 HCl

RN 600706-88-5 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-10-oxodecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

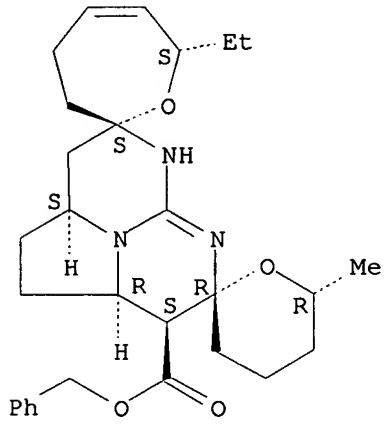
Absolute stereochemistry.



● 3 HCl

RN 732299-90-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, phenylmethyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

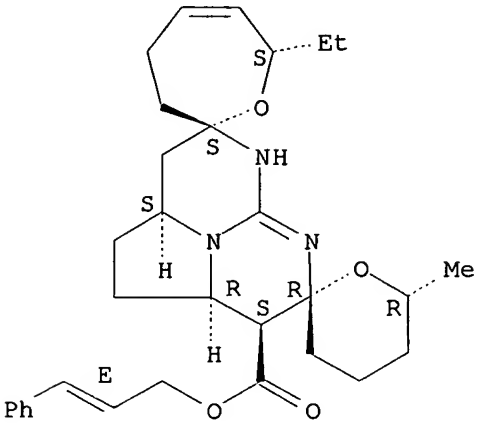
Absolute stereochemistry.



● HCl

RN 799812-00-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

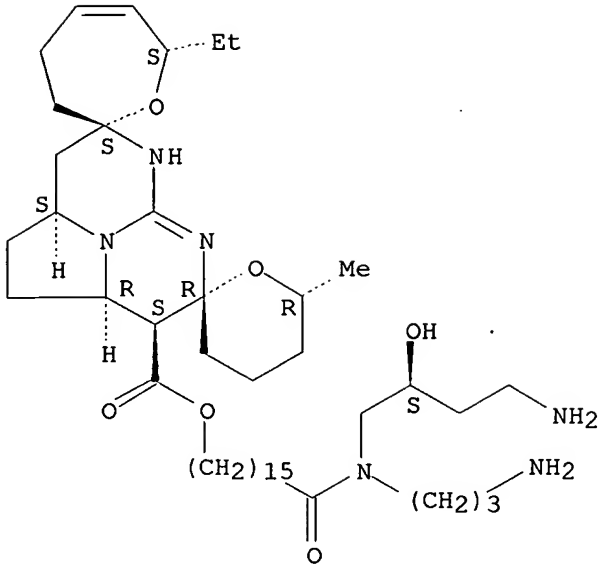


● HCl

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:824387 CAPLUS
DN 142:126838
TI Erythroid differentiation in K562 chronic myelogenous cells induced by crambescidin 800, a pentacyclic guanidine alkaloid
AU Aoki, Shunji; Kong, Dexin; Matsui, Kouhei; Kobayashi, Motomasa
CS Graduate School of Pharmaceutical Sciences, Osaka University, Suita, 565-0871, Japan
SO Anticancer Research (2004), 24(4), 2325-2330
CODEN: ANTRD4; ISSN: 0250-7005
PB International Institute of Anticancer Research
DT Journal
LA English
AB The differentiation induction of K562 chronic myelogenous leukemia (CML) cells by crambescidin 800, a pentacyclic guanidine alkaloid isolated from a marine sponge, was examined Crambescidin 800 increased Hb production in K562 cells at concns. of 0.15-1 μM and arrested the cell cycle of K562 cells at the S-phase. The expression of p21 was detected after 24-h treatment with crambescidin 800, and an increase of the expression was observed after 48-h treatment, but there was no remarkable change in the expression level of p27. This evidence indicates that crambescidin 800 induced the differentiation of K562 cells into erythroblasts accompanied by cell cycle arrest at the S-phase. Furthermore, crambescidin 800 induced a morphol. change with neurite outgrowth in Neuro 2A cells at a 0.03-0.1 μm concentration
IT 135257-46-4, Crambescidin 800
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(erythroid differentiation in K562 chronic myelogenous leukemia cells induced by pentacyclic guanidine alkaloid)
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8''-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

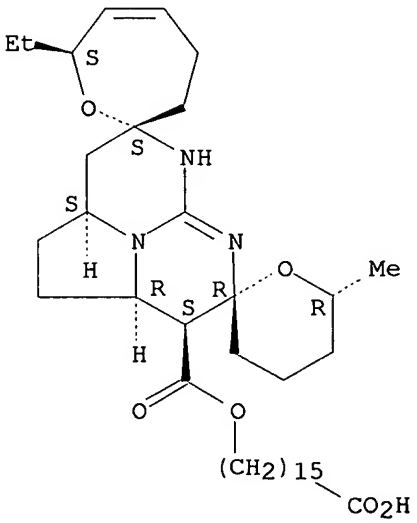
Absolute stereochemistry. Rotation (-).



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:465489 CAPLUS
DN 141:174351
TI Synthesis and anticancer activity of side chain analogs of the crambescidin alkaloids
AU Aron, Zachary D.; Pietraszkiewicz, Halina; Overman, Larry E.; Valeriote, Fredrick; Cuevas, Carman
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(13), 3445-3449
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 141:174351
AB Twenty three side chain analogs of the crambescidin alkaloids were prepared from the corresponding pentacyclic zwitterionic core acid. In the crambescidin 800 and 657 series, potency increased with increasing chain length. In addition, substantial variations in tumor selectivity with structure were seen. Crambescidin analogs having short, nonpolar side chains were identified for the first time as promising anticancer agents.
IT 214215-58-4, Crambescidin 657 214215-60-8, 13,14,15-Isocrambescidin 657 246851-97-8 275808-03-2 317831-97-3 600714-11-2 732299-89-7 732299-93-3 732299-96-6
RL: PAC (Pharmacological activity); BIOL (Biological study)
(anticancer activity of)
RN 214215-58-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

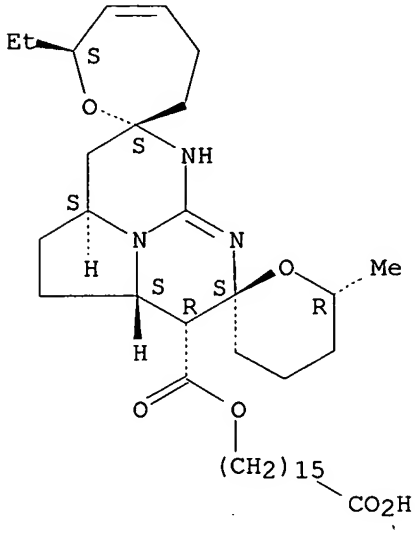
Absolute stereochemistry. Rotation (-).



RN 214215-60-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8'

,8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

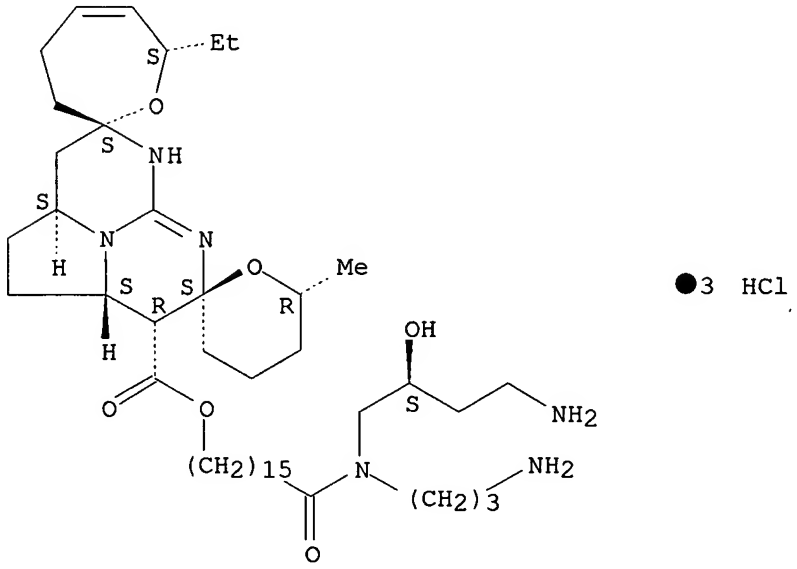
Absolute stereochemistry. Rotation (-).



RN 246851-97-8 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



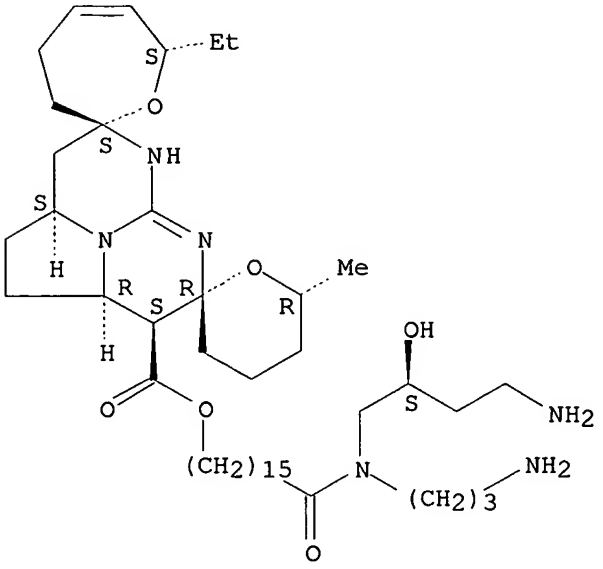
●3 HCl

RN 275808-03-2 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

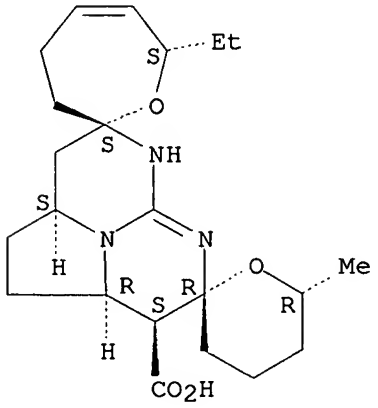


● 3 HCl

RN 317831-97-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

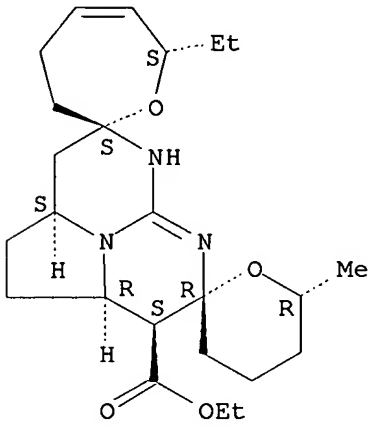


● HCl

RN 600714-11-2 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, ethyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

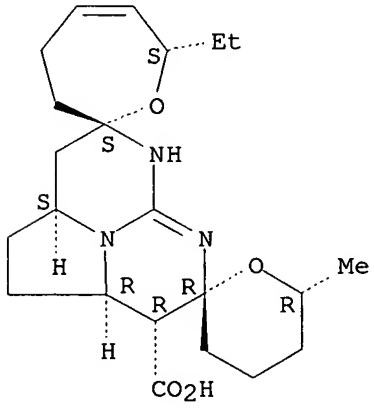
Absolute stereochemistry. Rotation (-).



● HCl

RN 732299-89-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

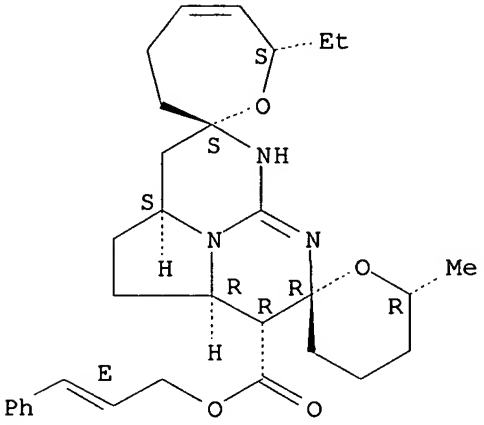


● HCl

RN 732299-93-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)- (9CI) (CA INDEX NAME)

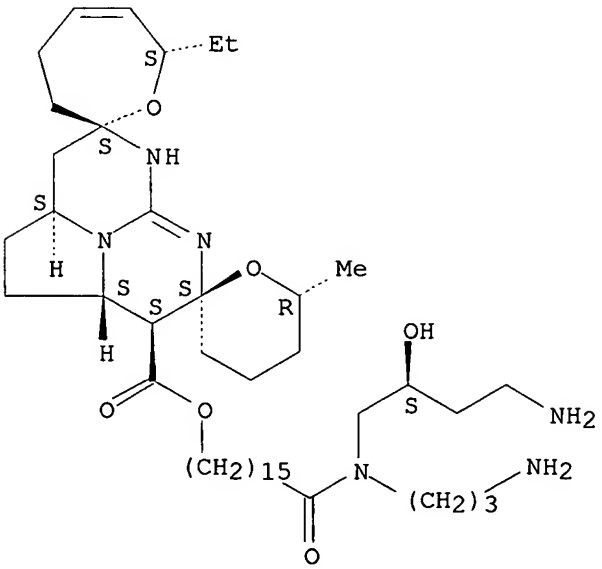
Absolute stereochemistry.
Double bond geometry as shown.



● HCl

RN 732299-96-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



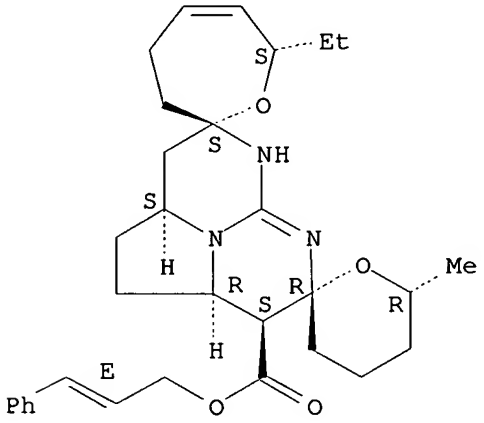
●3 HCl

IT 600707-02-6
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(synthesis and anticancer activity of side chain analogs of crambescidin alkaloids)
RN 600707-02-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

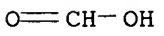
CRN 600706-77-2
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



CM 2

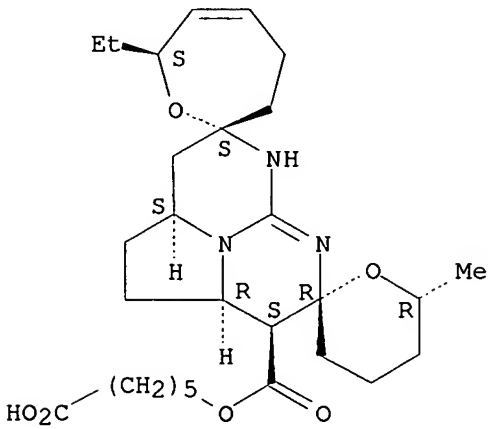
CRN 64-18-6
CMF C H2 O2



IT 600706-81-8P 600706-93-2P 600706-98-7P
600706-99-8P 600707-01-5P 732299-94-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and anticancer activity of side chain analogs of crambescidin alkaloids)
RN 600706-81-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 5-carboxypentyl ester,

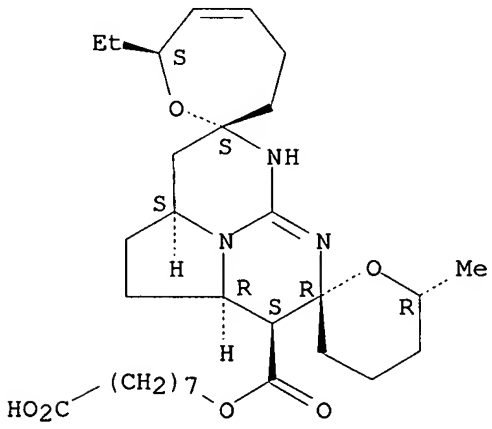
(2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



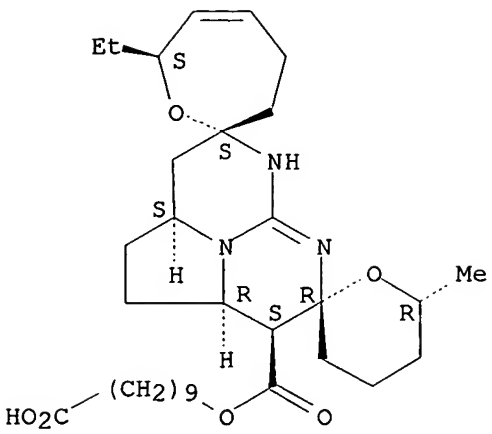
RN 600706-93-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 7-carboxyheptyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



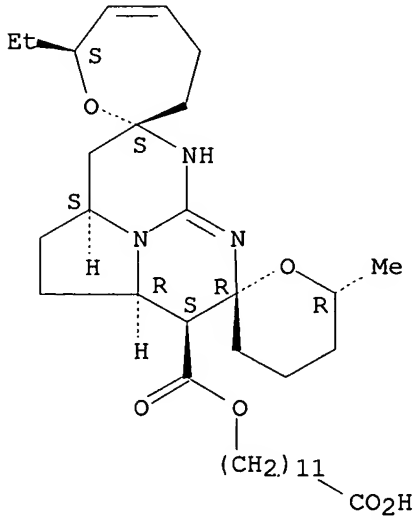
RN 600706-98-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 9-carboxynonyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



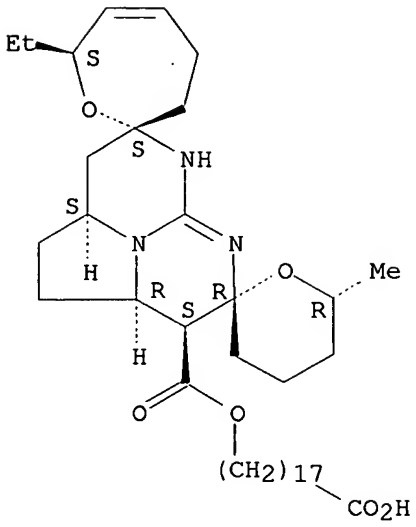
RN 600706-99-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 11-carboxyundecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



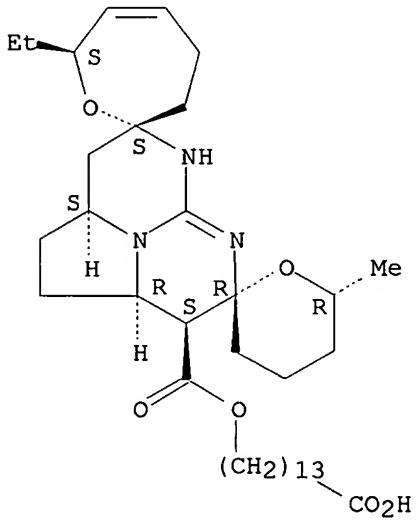
RN 600707-01-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 17-carboxyheptadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 732299-94-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 13-carboxytridecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

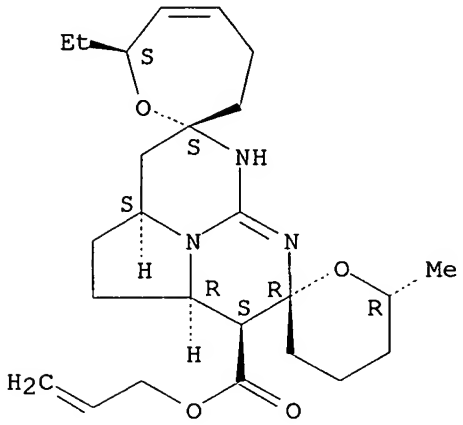
Absolute stereochemistry.



IT 316831-29-5P 600706-83-0P 600706-87-4P
600706-88-5P 600706-89-6P 600706-91-0P
732299-90-0P 732299-91-1P 732299-92-2P
732299-95-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and anticancer activity of side chain analogs of crambescidin alkaloids)
RN 316831-29-5 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 2-propenyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

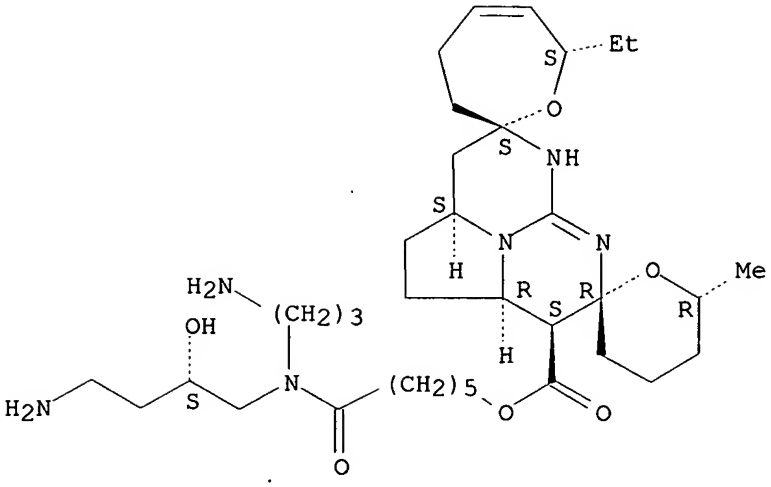


● HCl

RN 600706-83-0 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-6-oxohexyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

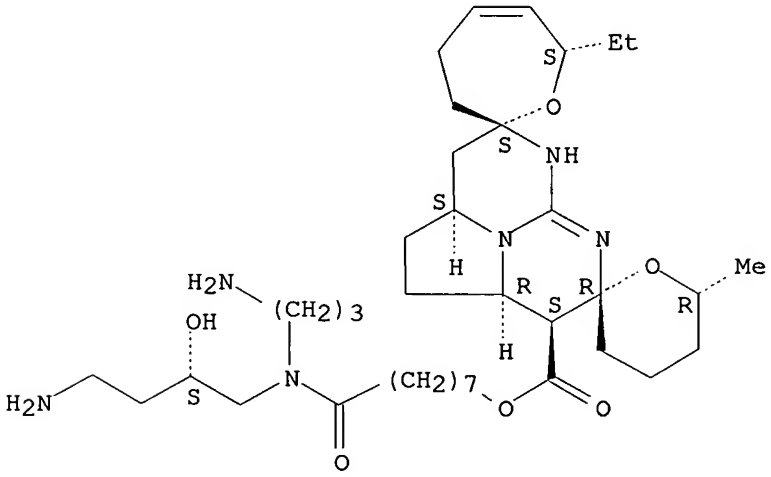
Absolute stereochemistry.



●3 HCl

RN 600706-87-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 8-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-8-oxooctyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

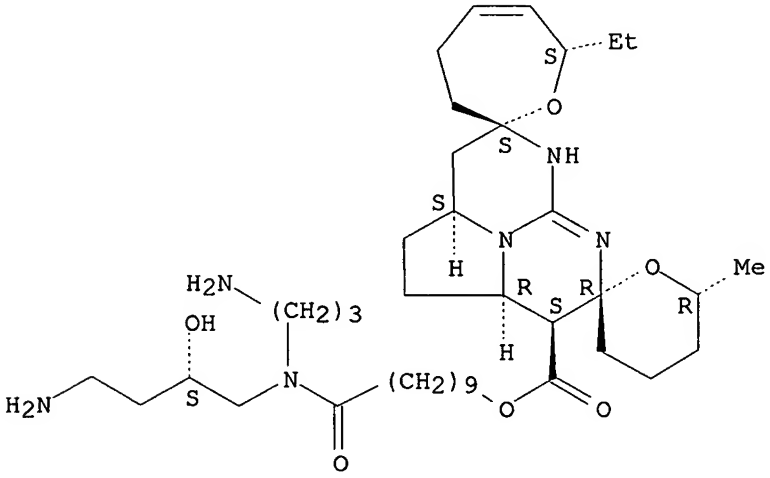


●3 HCl

RN 600706-88-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-10-oxodecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

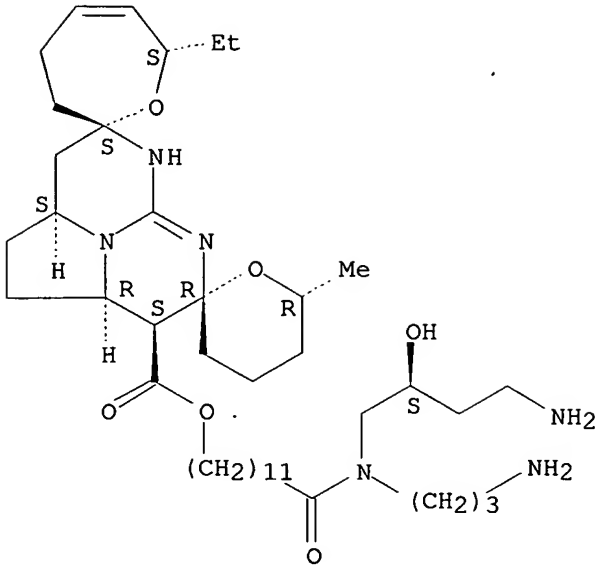


●3 HCl

RN 600706-89-6 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 12-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-12-oxododecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

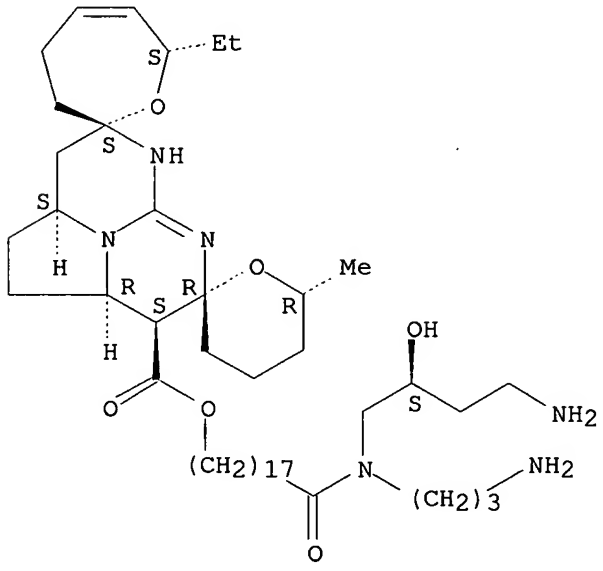
Absolute stereochemistry.



●3 HCl

RN 600706-91-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-18-oxooctadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

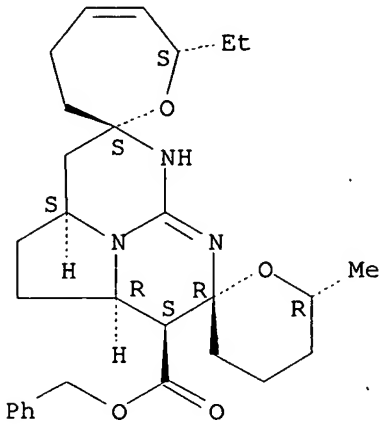


●3 HCl

RN 732299-90-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, phenylmethyl ester, monohydrochloride,

(2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

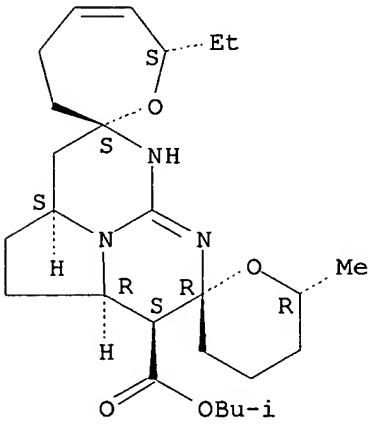
Absolute stereochemistry.



● HCl

RN 732299-91-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 2-methylpropyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

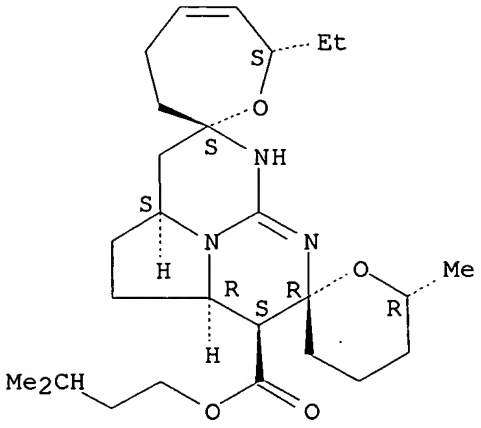


● HCl

RN 732299-92-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 3-methylbutyl ester, monohydrochloride,

(2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

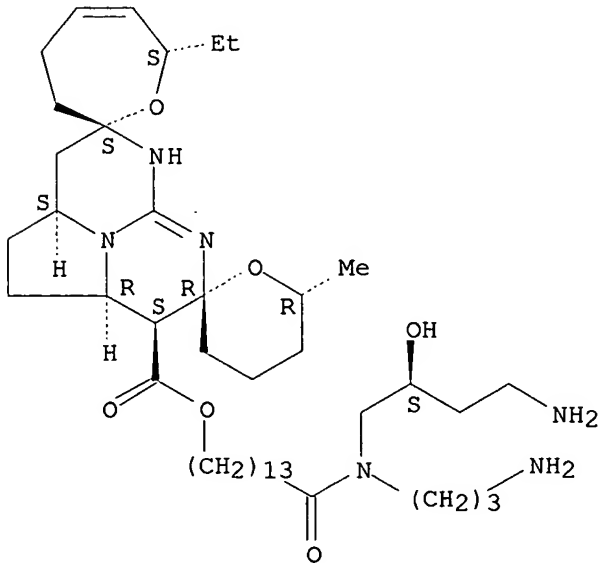
Absolute stereochemistry.



● HCl

RN 732299-95-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 14-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-14-oxotetradecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●3 HCl

IT 600706-82-9P 600707-03-7P 600707-05-9P
600707-06-0P 600707-08-2P 732299-97-7P

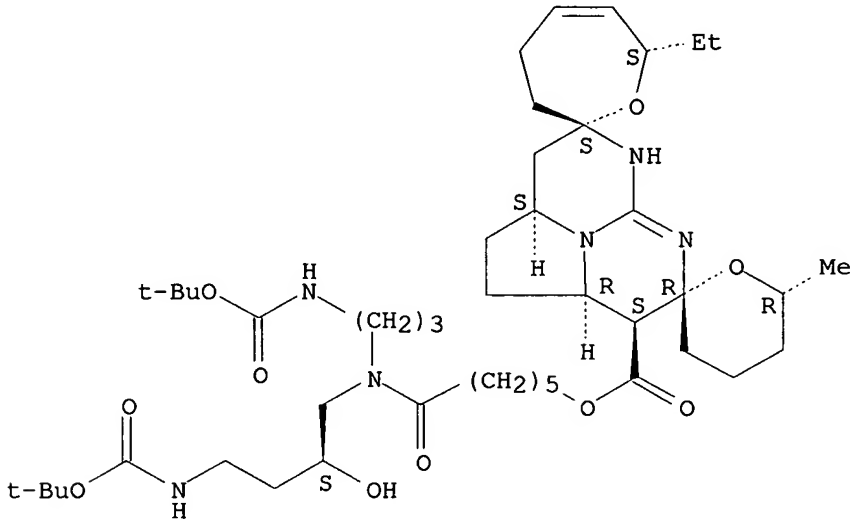
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and anticancer activity of side chain analogs of crambescidin alkaloids)

RN 600706-82-9 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-6-oxohexyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

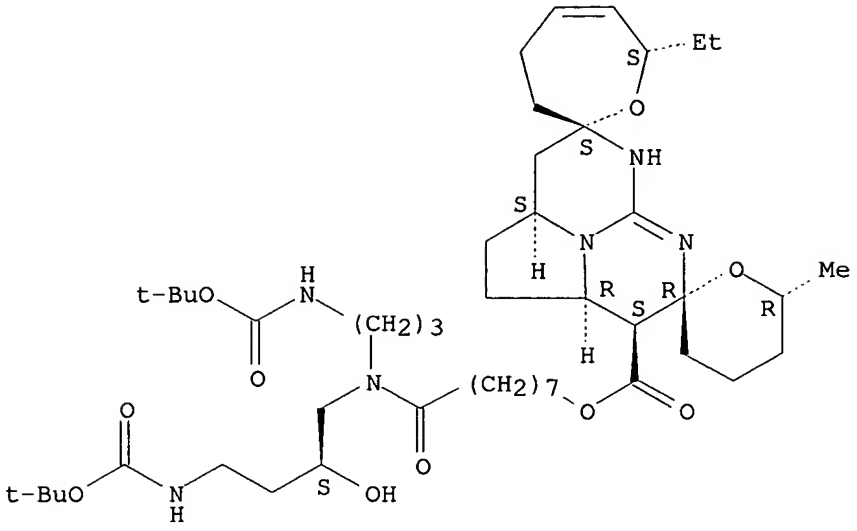
● HCl

RN 600707-03-7 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 8-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-8-oxooctyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



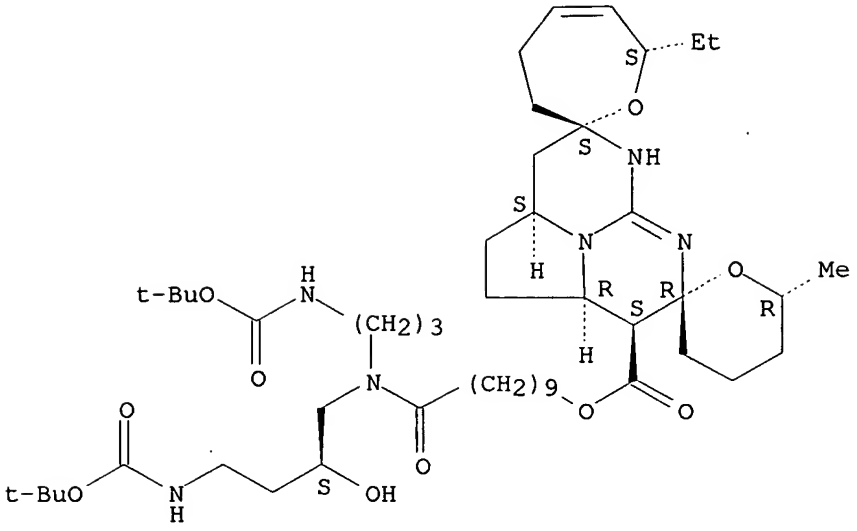
PAGE 2-A

● HCl

RN 600707-05-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-10-oxodecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



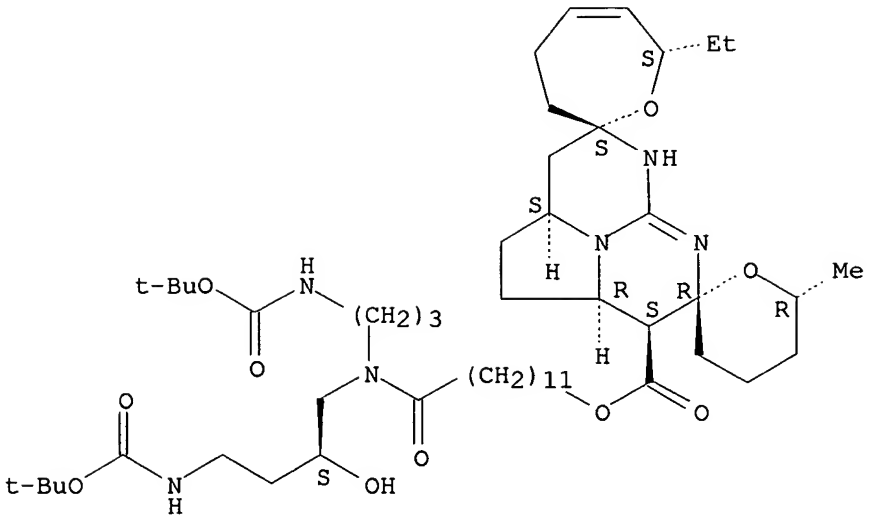
PAGE 2-A

● HCl

RN 600707-06-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 12-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-12-oxododecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

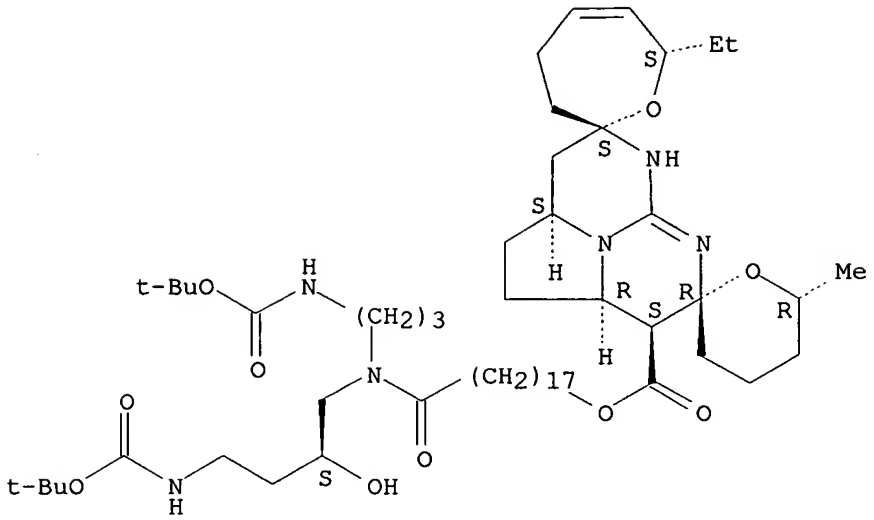
● HCl

RN 600707-08-2 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-18-oxooctadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



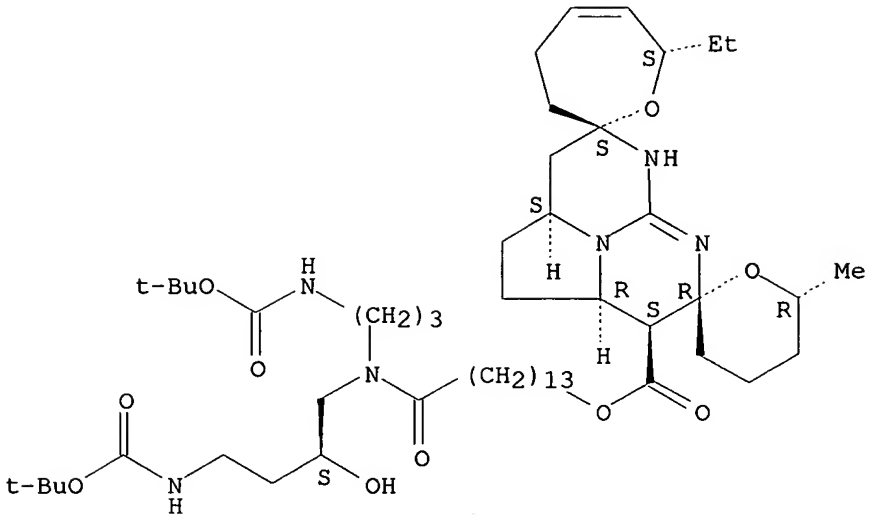
PAGE 2-A

● HCl

RN 732299-97-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 14-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-14-oxotetradecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



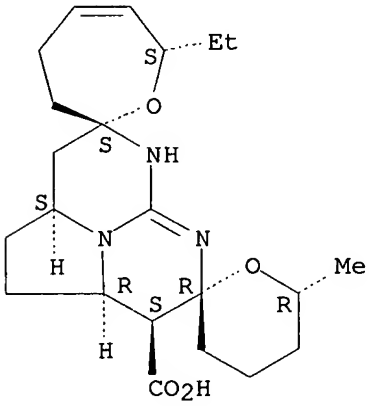
PAGE 2-A

● HCl

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:465166 CAPLUS
DN 141:120455
TI Monanchorin, a bicyclic alkaloid from the sponge Monanchora ungiculata
AU Meragelman, Karina M.; McKee, Tawnya C.; McMahon, James B.
CS Molecular Targets Development Program, Center for Cancer Research, National Cancer Institute at Frederick, Frederick, MD, 21702-1201, USA
SO Journal of Natural Products (2004), 67(7), 1165-1167
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
AB Monanchorin (I), a guanidine alkaloid with an unusual bicyclic skeleton, together with the known pentacyclic alkaloid crambescidin acid have been isolated from the aqueous extract of the sponge Monanchora ungiculata.
IT 147664-30-0, Crambescidin acid
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(bicyclic alkaloid from sponge Monanchora ungiculata)
RN 147664-30-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

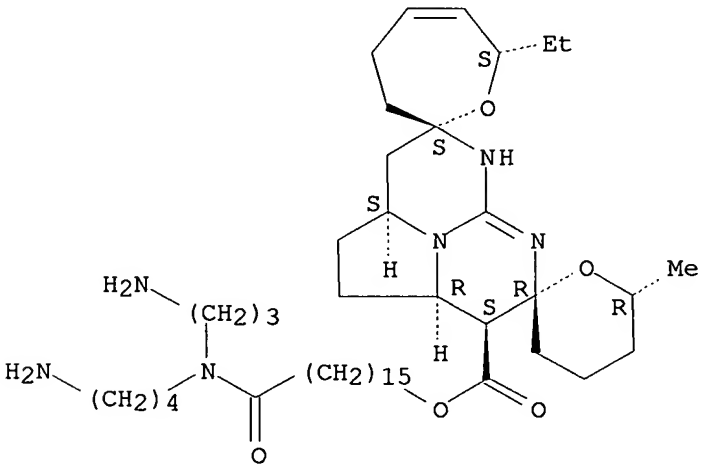
Absolute stereochemistry.



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

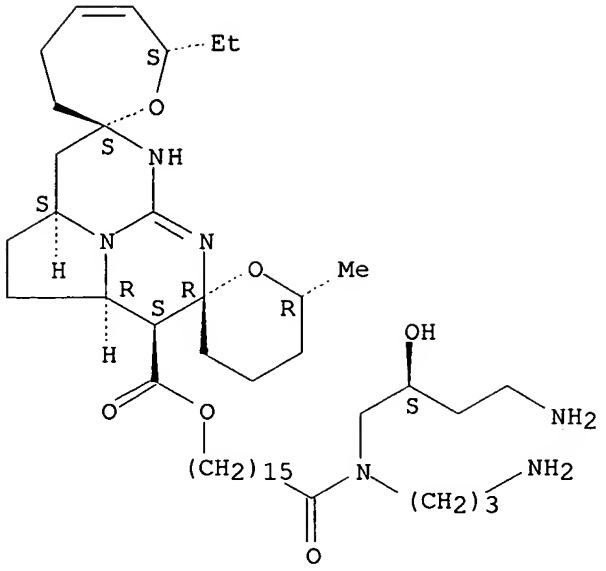
L11 ANSWER 9 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:74641 CAPLUS
DN 140:339505
TI The tethered Biginelli condensation in natural product synthesis
AU Aron, Zachary D.; Overman, Larry E.
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Chemical Communications (Cambridge, United Kingdom) (2004), (3), 253-265
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal; General Review
LA English
AB This review describes the development of the tethered Biginelli condensation and its application to the total synthesis of structurally complex, bioactive guanidine alkaloids.
IT 124512-47-6P, Ptilomycalin A 135257-46-4P, Crambescidin 800 151121-78-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(tethered Biginelli condensation in synthesis of guanidine alkaloids)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



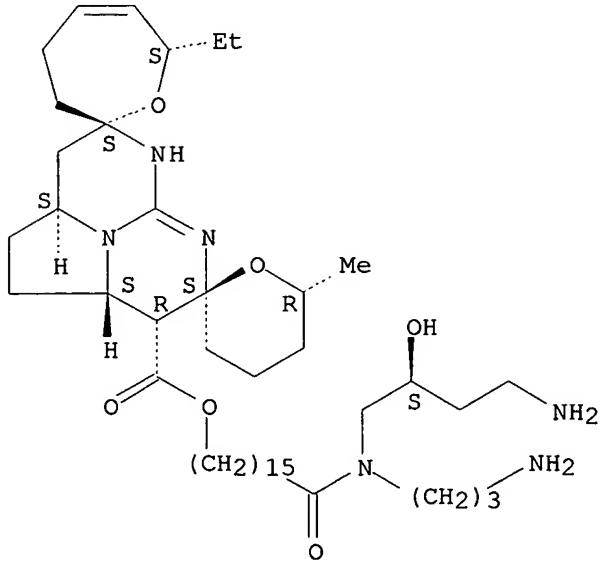
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 151121-78-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)-(9CI) (CA INDEX NAME)

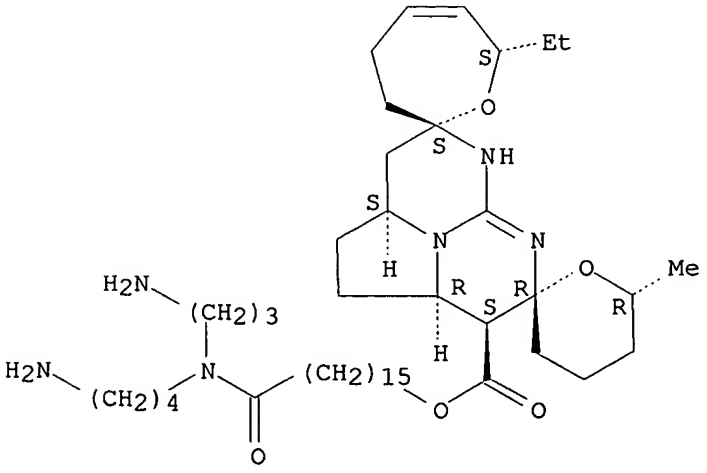
Absolute stereochemistry. Rotation (-).



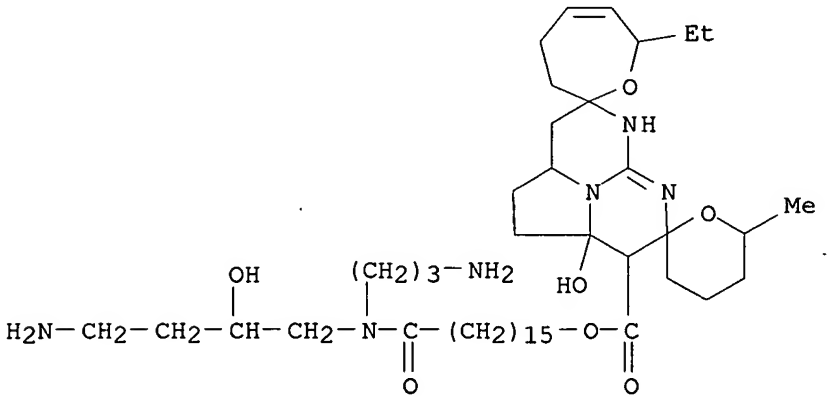
RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:975892 CAPLUS
DN 140:199483
TI Synthesis of marine guanidine alkaloids and their application as chemical/biological tools
AU Nagasawa, Kazuo; Hashimoto, Yuichi
CS Institute of Molecular and Cellular Biosciences, The University of Tokyo, Tokyo, 113-0032, Japan
SO Chemical Record (2003), 3(4), 201-211
CODEN: CRHEAK; ISSN: 1527-8999
PB John Wiley & Sons, Inc.
DT Journal; General Review
LA English
AB A review with refs. Ptilomycalin A and crambescidins, novel marine guanidine alkaloids, have a unique pentacyclic guanidine structure, and exhibit a considerable array of biol. activities. The first method developed for the synthesis of the pentacyclic guanidine core structure involved successive 1,3-dipolar cycloaddn. reactions and resulted in the first total synthesis of crambescidin 359. The synthesis of other pentacyclic guanidine derivs. has been based on this methodol. and applied as tools for studying biol. activities, and as chemical reaction catalysts.
IT 124512-47-6P, Ptilomycalin A 135257-45-3P, Crambescidin 816 135257-46-4P, Crambescidin 800 135257-47-5P, Crambescidin 830 135283-73-7P, Crambescidin 844 151121-78-7P, Isocrambescidin 800 163597-72-6P, Celeromycalin 163597-73-7P, Fromiamycalin
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis of marine guanidine alkaloids and their application as chemical/biol. tools)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

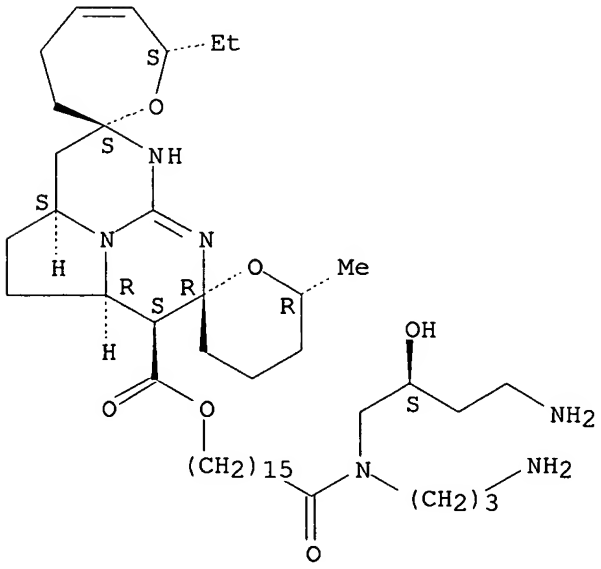


RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



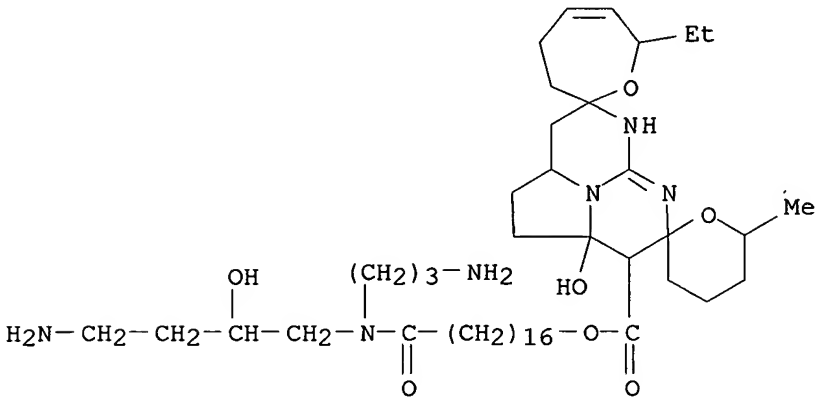
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



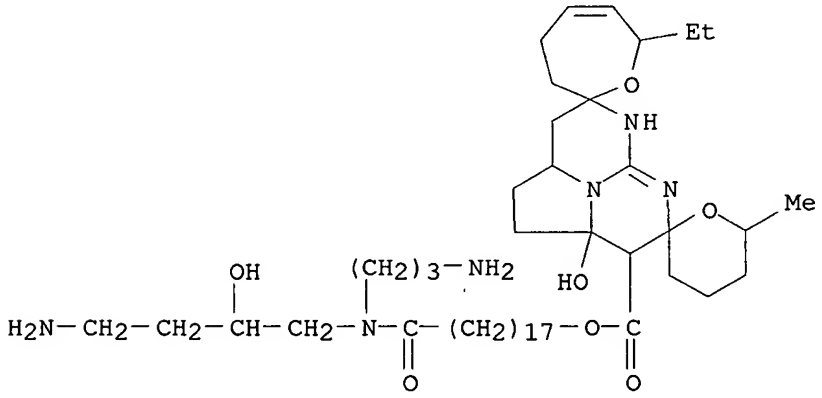
RN 135257-47-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8'

,8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 17-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-17-oxoheptadecyl ester (9CI) (CA INDEX NAME)



RN 135283-73-7 CAPLUS

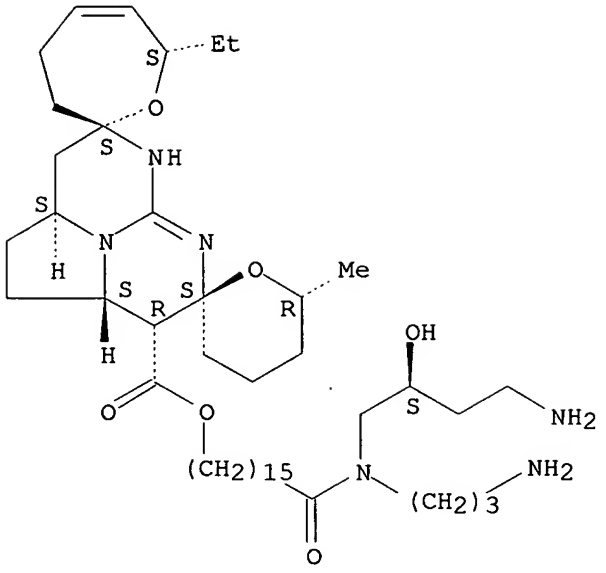
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 18-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-18-oxooctadecyl ester (9CI) (CA INDEX NAME)



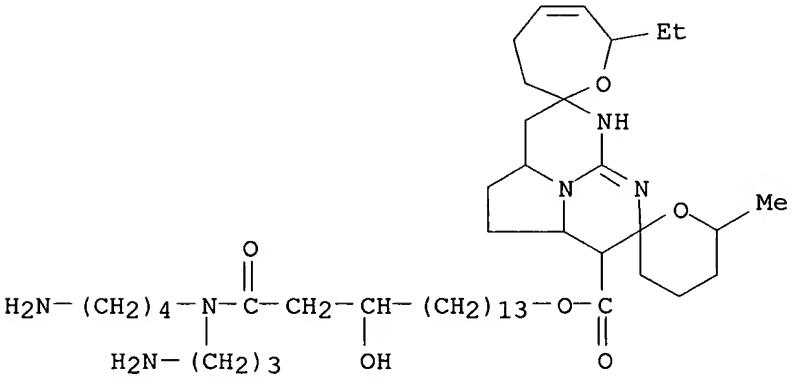
RN 151121-78-7 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

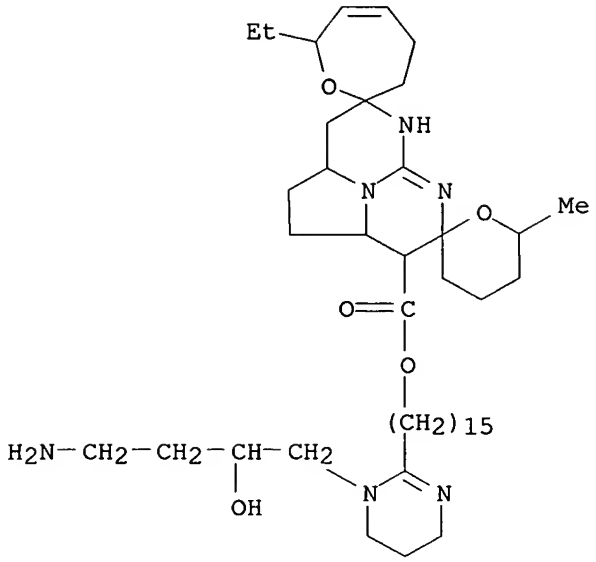
Absolute stereochemistry. Rotation (-).



RN 163597-72-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (14R)-16-[(4-aminobutyl)(3-aminopropyl)amino]-14-hydroxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)



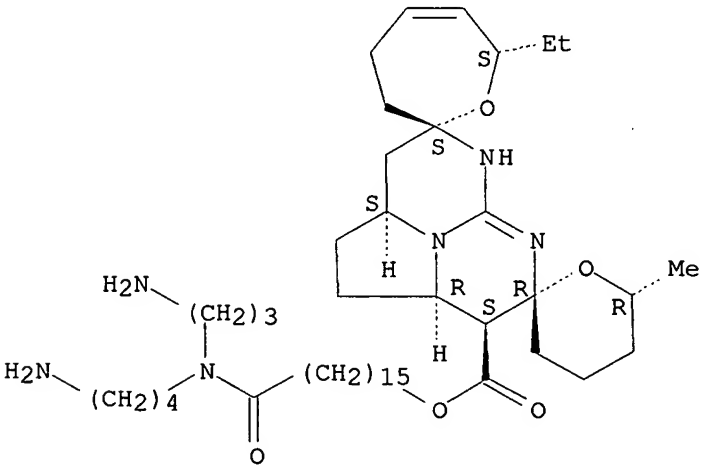
RN 163597-73-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-[1-(4-amino-2-hydroxybutyl)-1,4,5,6-tetrahydro-2-pyrimidinyl]pentadecyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β(R*),8'aα]]- (9CI) (CA INDEX NAME)



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:949253 CAPLUS
DN 140:300638
TI A new bicyclic guanidine alkaloid, Sch 575948, from a marine sponge, Ptilocaulis spiculifer
AU Yang, Shu-wei; Chan, Tze-ming; Pomponi, Shirley A.; Chen, Guodong; Wright, Amy E.; Patel, Mahesh; Gullo, Vincent; Pramanik, Birendra; Chu, Min
CS Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA
SO Journal of Antibiotics (2003), 56(11), 970-972
CODEN: JANTAJ; ISSN: 0021-8820
PB Japan Antibiotics Research Association
DT Journal
LA English
AB A new antibacterial compound Sch 575948 (I) was isolated along with a known alkaloid ptilomycalin A from a marine sponge Ptilocaulis spiculifer as a part of a continuing search for novel anti-microbial agents. Sch 575948 was identified as a bicyclic bis-guanidine type of alkaloid, a homolog of crambescin A, identified as a major component of the homolog complex. The identified structure of Sch 575948 is a new member of crambescin A class of compds. with a shorter alkyl side chain. Sch 575948 exhibited antibacterial activity against a super sensitive strain of Staphylococcus aureus.
IT 124512-47-6, Ptilomycalin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(bicyclic guanidine alkaloid from marine sponge Ptilocaulis spiculifer)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

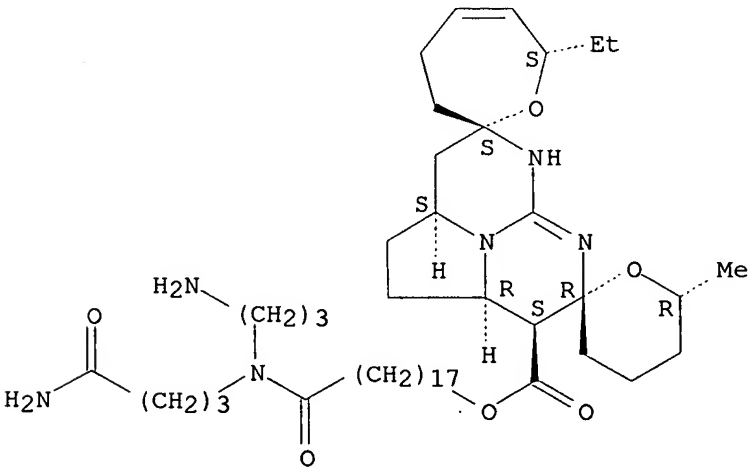
Absolute stereochemistry. Rotation (-).



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:832854 CAPLUS
DN 140:2958
TI Crambescidin 826 and dehydrocrambine A: New polycyclic guanidine alkaloids from the marine sponge Monanchora sp. that inhibit HIV-1 fusion
AU Chang, LengChee; Whittaker, Noel F.; Bewley, Carole A.
CS Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0820, USA
SO Journal of Natural Products (2003), 66(11), 1490-1494
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
AB Two new polycyclic guanidine alkaloids, crambescidin 826 (I) and dehydrocrambine A (II), and the known compds. crambescidin 800 (III) and fromiamycalin (IV) were isolated from the marine sponge Monanchora sp. The structures of I and II were elucidated by 2D NMR and mass spectrometry, and relative stereochem. was established by anal. of coupling consts. and ROESY spectra. The pentacyclic guanidine alkaloids I, III, and IV inhibit HIV-1 envelope-mediated fusion in vitro with IC50's of 1-3 μM, while compound II, a tricyclic guanidine alkaloid, showed weaker inhibition, with an IC50 of .apprx.35 μM.
IT 628727-32-2P, Crambescidine 826
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(polycyclic guanidine alkaloids from marine sponge Monanchora sp. that inhibit HIV-1 fusion)
RN 628727-32-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[(4-amino-4-oxobutyl)(3-aminopropyl)amino]-18-oxooctadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



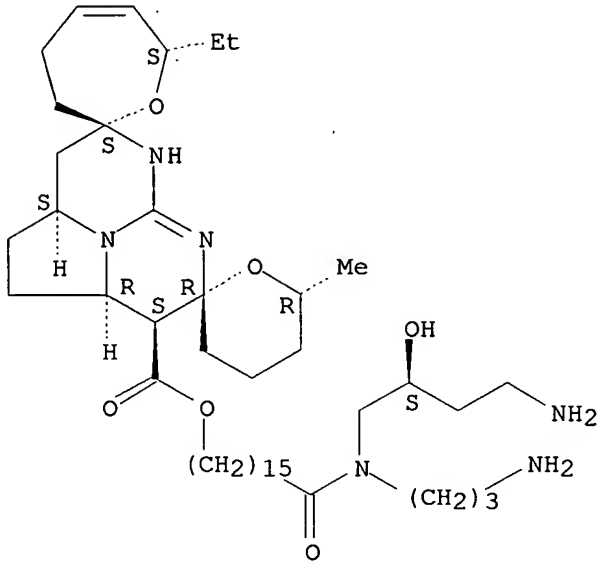
IT 135257-46-4, Crambescidin 800 163597-73-7, Fromiamycalin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(polycyclic guanidine alkaloids from marine sponge Monanchora sp. that inhibit HIV-1 fusion)

RN 135257-46-4 CAPLUS

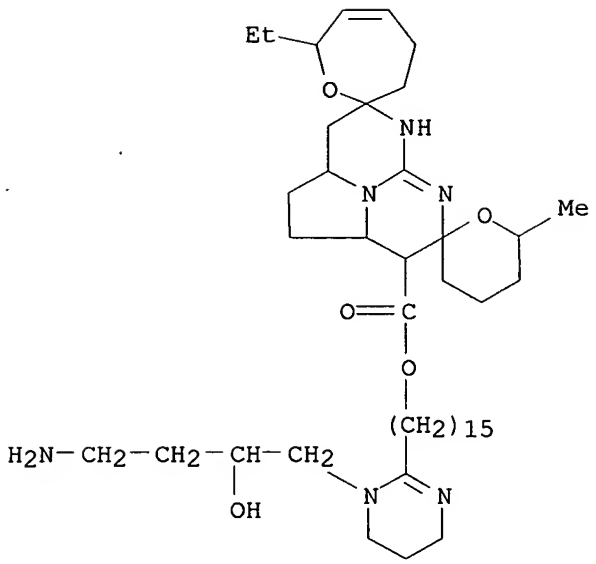
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 163597-73-7 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-[1-(4-amino-2-hydroxybutyl)-1,4,5,6-tetrahydro-2-pyrimidinyl]pentadecyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β(R*),8'aα]]- (9CI)
(CA INDEX NAME)



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:737413 CAPLUS
DN 139:261451
TI Preparation of crambescidin core acid intermediates and their use for preparing crambescidin alkaloid analogs as antiviral, antifungal and/or antitumor agents
IN Overman, Larry E.; Stappenbeck, Frank; McDonald, Andrew I.; Aron, Zachary D.
PA The Regents of the University of California, USA
SO U.S. Pat. Appl. Publ., 29 pp., Cont.-in-part of U.S. Ser. No. 18,630.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2003176697	A1	20030918	US 2002-255994	20020924
WO 2001000626	A1	20010104	WO 2000-US18395	20000630
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ZA 2001010327	A	20030314	ZA 2001-10327	20011214
WO 2004028452	A2	20040408	WO 2003-US29888	20030923
WO 2004028452	A3	20040521		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003282807	A1	20040419	AU 2003-282807	20030923

PRAI US 1999-142027P P 19990630
US 1999-142028P P 19990630
WO 2000-US18395 W 20000630
US 2001-18630 A2 20011214
US 2002-255994 A 20020924
WO 2003-US29888 W 20030923

OS MARPAT 139:261451

AB The invention provides methods to synthesize zwitterionic pentacyclic crambescidin core intermediates having the carboxylate side chain in the natural axial orientation, such as I [R1 = saturated, unsatd., cyclic, acyclic, straight, branched chiral and achiral hydrocarbyl group; R2 = H, alkyl, aryl, heteroaryl, carboxy, carboxylate anion, phosphonate, phosphate, sulfonate, sulfate, borate, boronate, amine], and a range of crambescidin alkaloid analogs for their therapeutic use as antiviral, antifungal and/or antitumor agents. Thus, crambescidin 657 analog II was prepared via a multistep synthetic sequence starting from cinnamyl alc., Me (7R)-7-(tert-butyldimethylsilyl)-3-oxo-octanoate, (6S,11Z,13S)-8-(1',3'-dioxan-2'-yl)-2-methyl-13-triisopropylsilyloxy-6-ureidopentadeca-2,11-

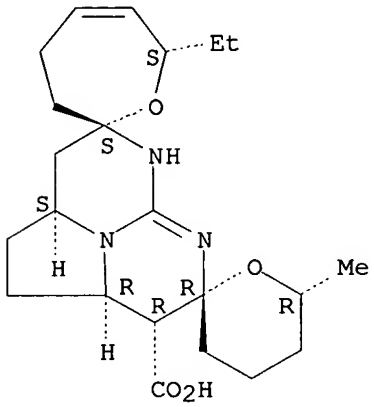
diene and allyl 6-iodohexanoate. The prepared compds. were evaluated for in vitro cytotoxicity against murine tumor (e.g., colon 38 tumor, or as a single cell from a murine leukemia (L1210) cell line).

IT 317831-93-9P 600706-81-8P 600706-93-2P
600706-98-7P 600706-99-8P 600707-00-4P
600707-01-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of crambescidin core acid intermediates and their use for preparing crambescidin alkaloid analogs as antiviral, antifungal and/or antitumor agents)

RN 317831-93-9 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)- (9CI) (CA INDEX NAME)

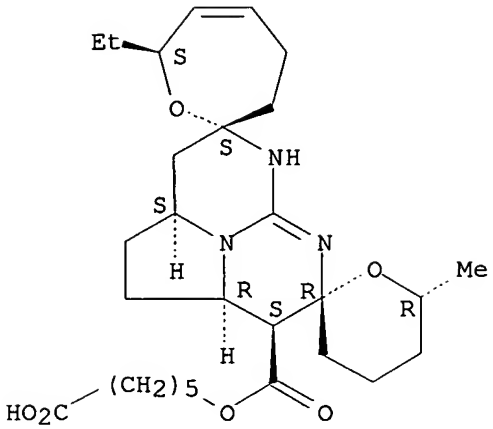
Absolute stereochemistry.



RN 600706-81-8 CAPLUS

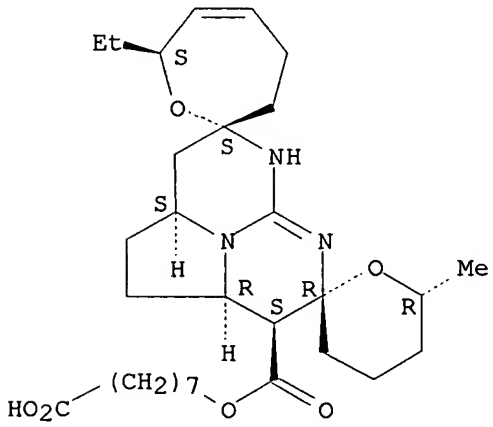
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 5-carboxypentyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



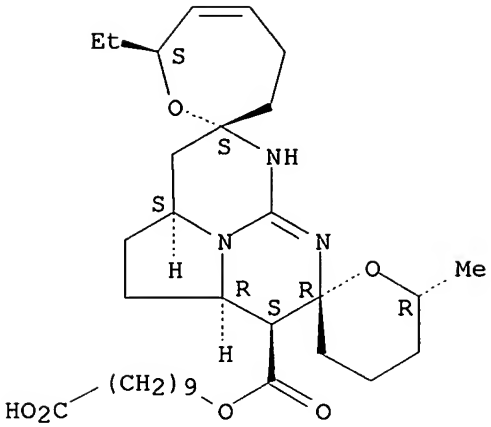
RN 600706-93-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 7-carboxyheptyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



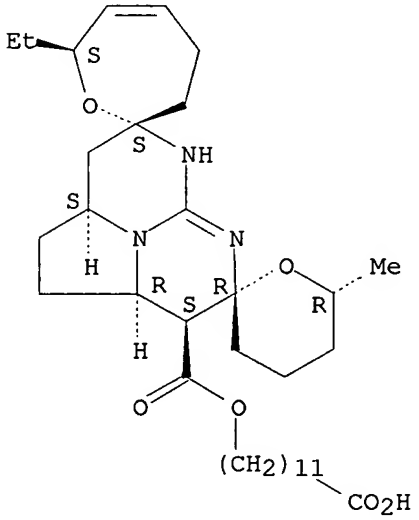
RN 600706-98-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 9-carboxynonyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



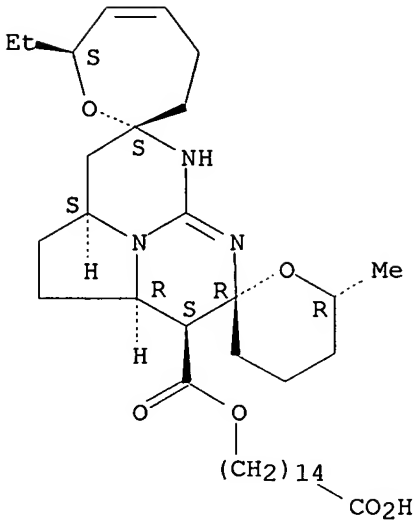
RN 600706-99-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 11-carboxyundecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



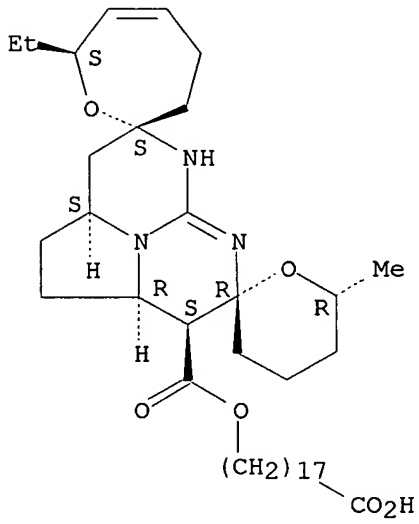
RN 600707-00-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 14-carboxytetradecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 600707-01-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 17-carboxyheptadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



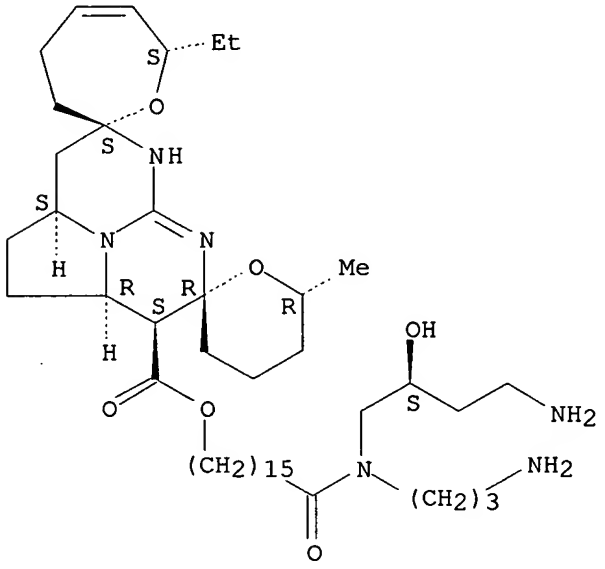
IT 135257-46-4DP, Crambescidin 800, analog 214215-58-4DP, Crambescidin 657, analogs 600706-80-7P 600706-83-0P 600706-86-3P 600706-87-4P 600706-88-5P 600706-89-6P 600706-90-9P 600706-91-0P 600714-11-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of crambescidin core acid intermediates and their use for

preparing crambescidin alkaloid analogs as antiviral, antifungal and/or antitumor agents)

RN 135257-46-4 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

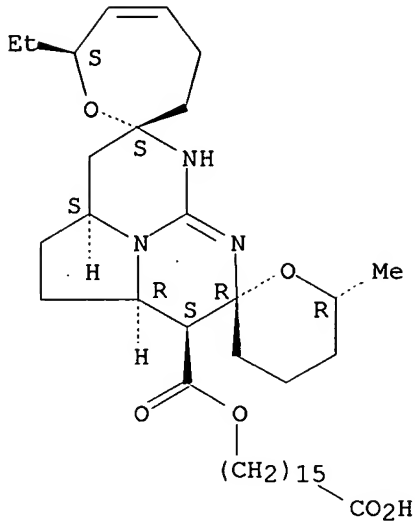
Absolute stereochemistry. Rotation (-).



RN 214215-58-4 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

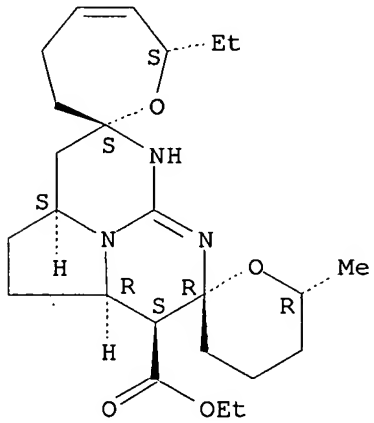


RN 600706-80-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, ethyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

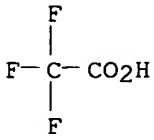
CRN 600706-79-4
CMF C24 H37 N3 O4

Absolute stereochemistry. Rotation (-).



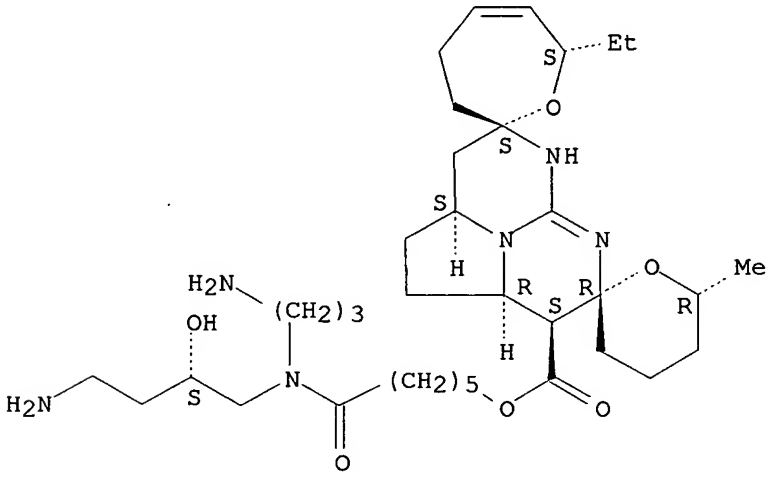
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 600706-83-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-6-oxohexyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



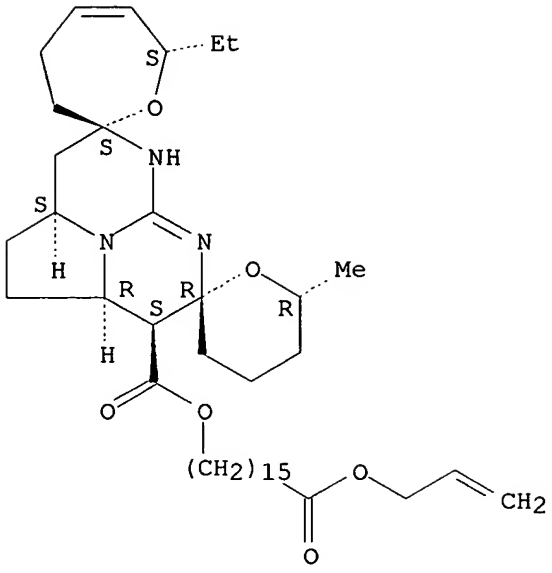
●3 HCl

RN 600706-86-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

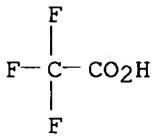
CRN 162145-89-3
CMF C41 H67 N3 O6

Absolute stereochemistry. Rotation (-).



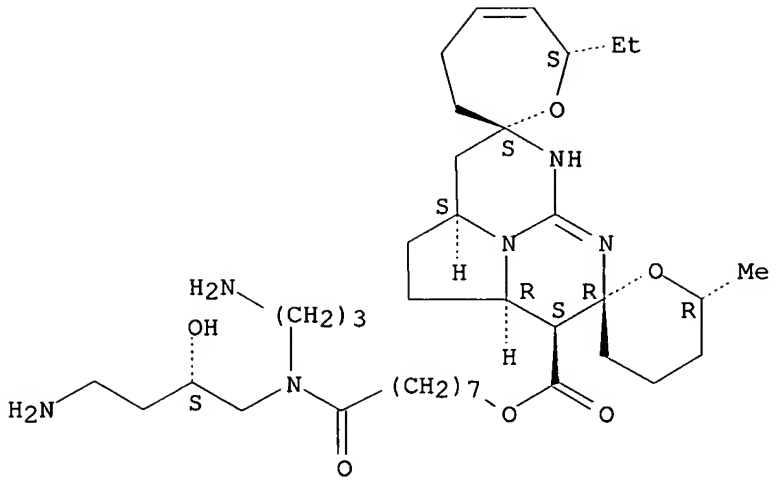
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 600706-87-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 8-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-8-oxooctyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

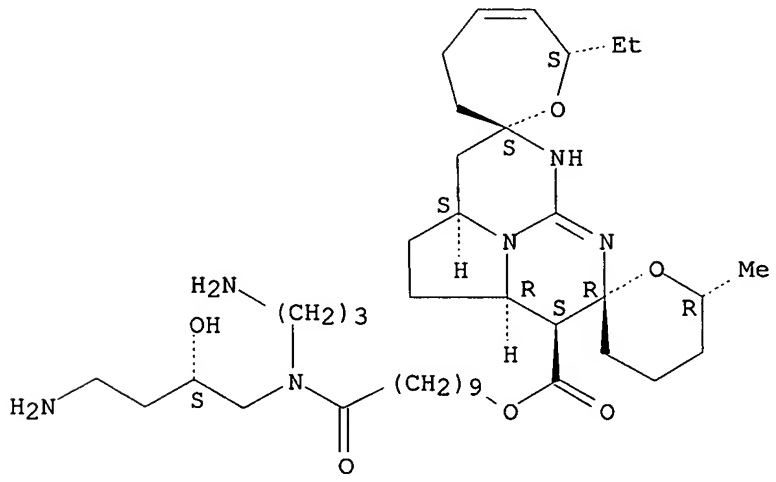
Absolute stereochemistry.



●3 HCl

RN 600706-88-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-10-oxodecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

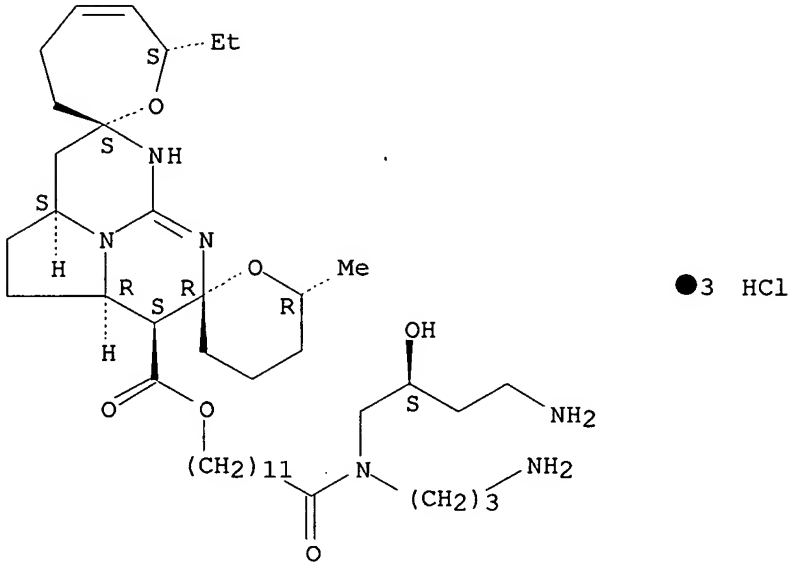


●3 HCl

RN 600706-89-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 12-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-12-oxododecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

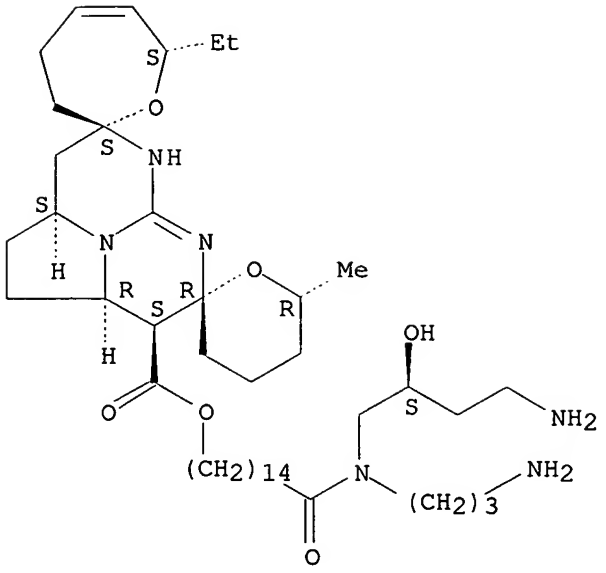
Absolute stereochemistry.



RN 600706-90-9 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-15-oxopentadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

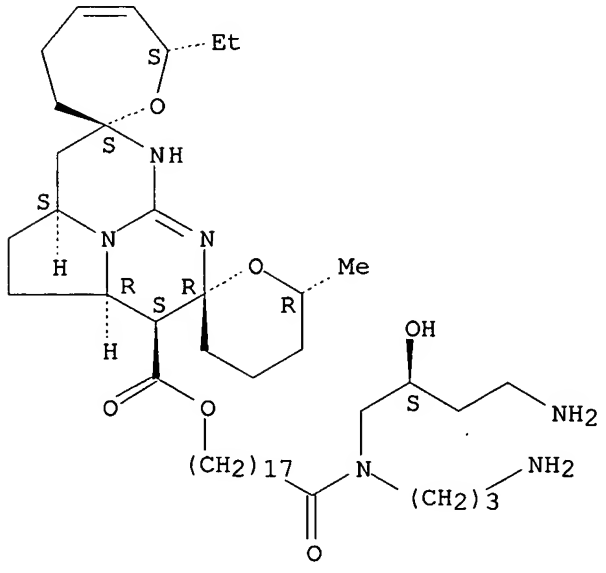
Absolute stereochemistry.



●3 HCl

RN 600706-91-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-18-oxooctadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

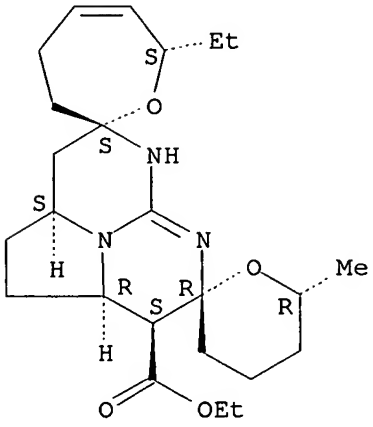


●3 HCl

RN 600714-11-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, ethyl ester, monohydrochloride,

(2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● HCl

IT 600708-86-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of crambescidin core acid intermediates and their use for preparing crambescidin alkaloid analogs as antiviral, antifungal and/or antitumor agents)

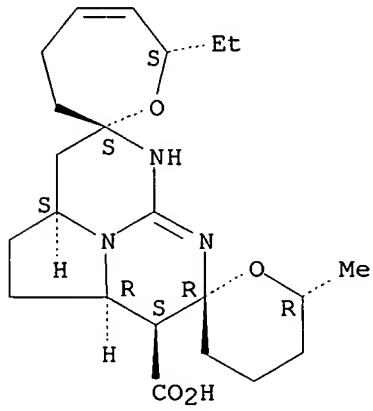
RN 600708-86-9 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'S,8'aR), compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147664-30-0
CMF C22 H33 N3 O4

Absolute stereochemistry.



CM 2

CRN 67-56-1
CMF C H4 O

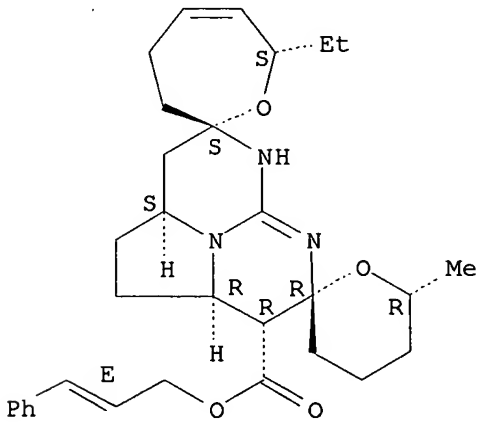
H_3C-OH

IT 600706-76-1P 600706-78-3P 600706-82-9P
600707-02-6P 600707-03-7P 600707-05-9P
600707-06-0P 600707-07-1P 600707-08-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of crambescidin core acid intermediates and their use for preparing crambescidin alkaloid analogs as antiviral, antifungal and/or antitumor agents)
RN 600706-76-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

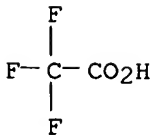
CRN 600706-75-0
CMF C31 H41 N3 O4

Absolute stereochemistry.
Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

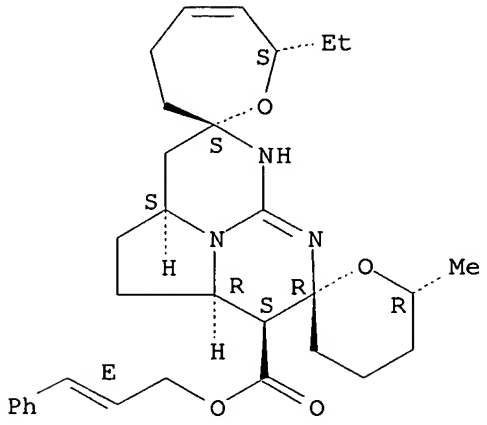


RN 600706-78-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

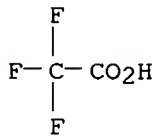
CRN 600706-77-2
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

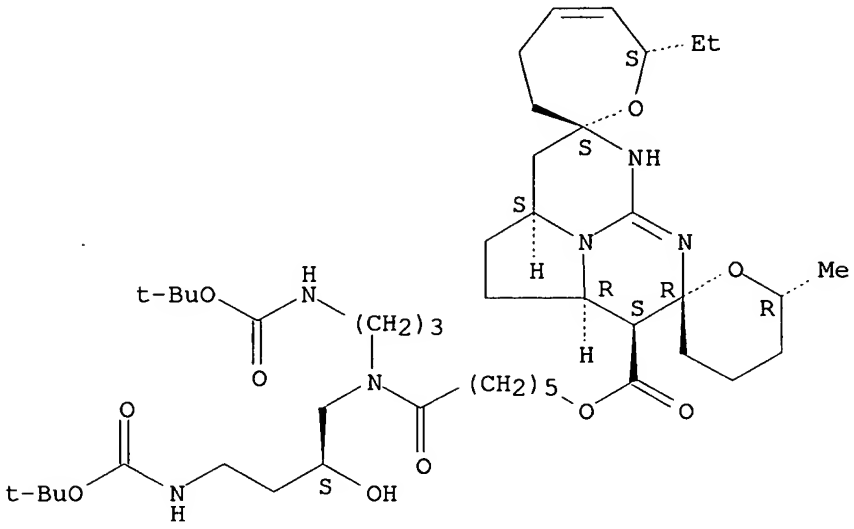


RN 600706-82-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 6-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-

dimethylethoxy)carbonyl]amino]propyl]amino]-6-oxohexyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

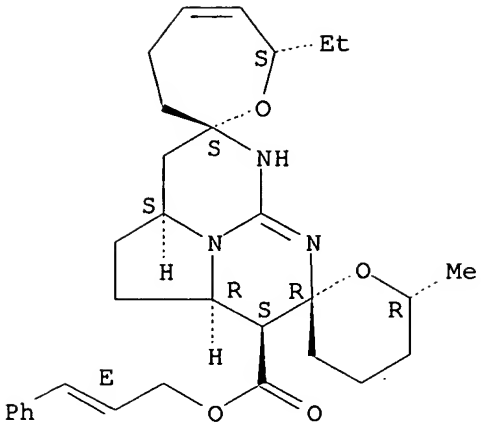
● HCl

RN 600707-02-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2E)-3-phenyl-2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

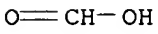
CRN 600706-77-2
CMF C31 H41 N3 O4

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



CM 2

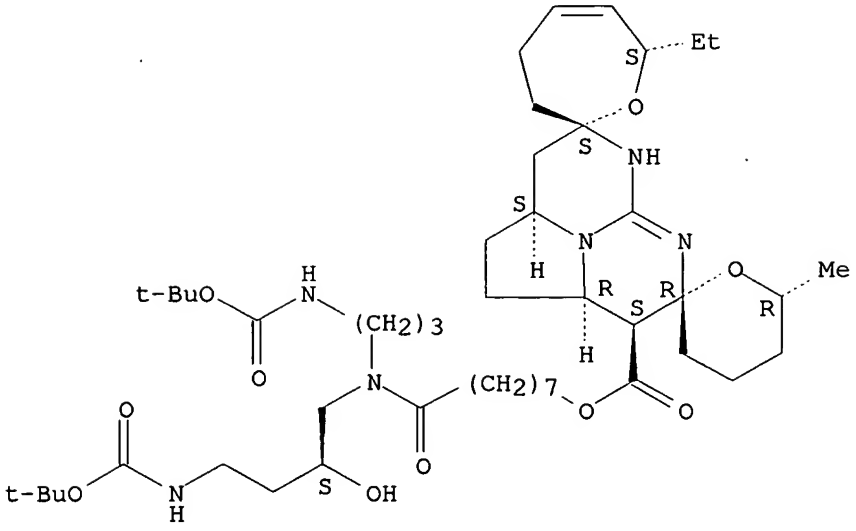
CRN 64-18-6
CMF C H2 O2



RN 600707-03-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 8-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-8-oxooctyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



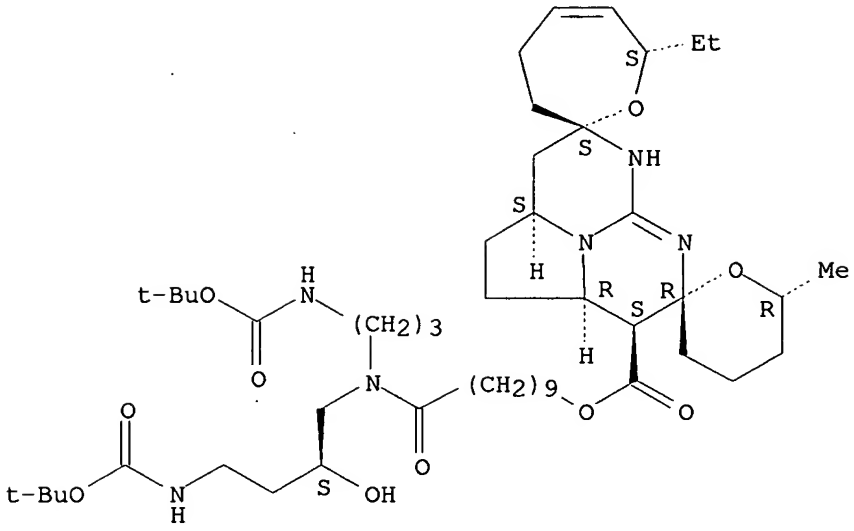
PAGE 2-A

● HCl

RN 600707-05-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 10-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-10-oxodecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



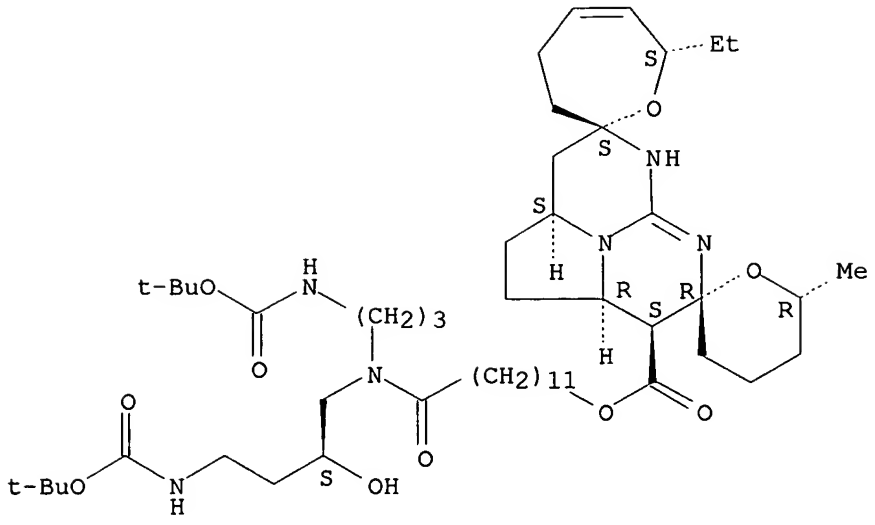
PAGE 2-A

● HCl

RN 600707-06-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 12-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-12-oxododecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



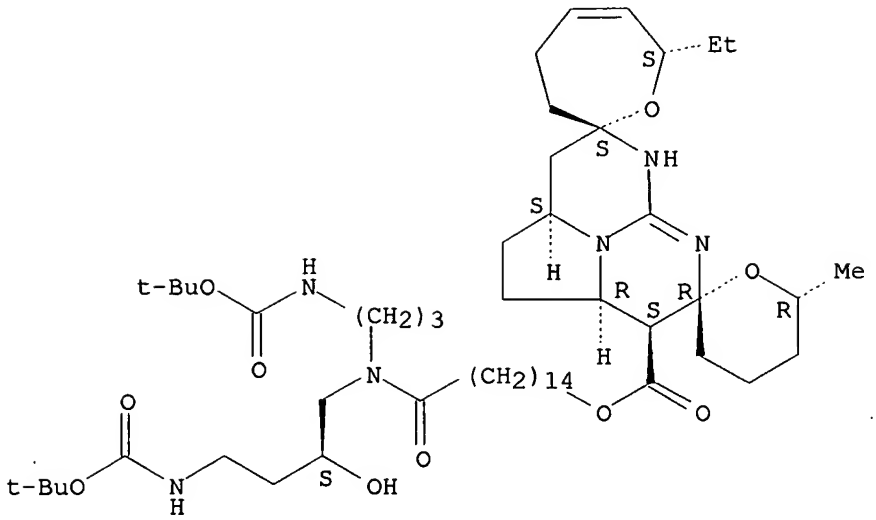
PAGE 2-A

● HCl

RN 600707-07-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-15-oxopentadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



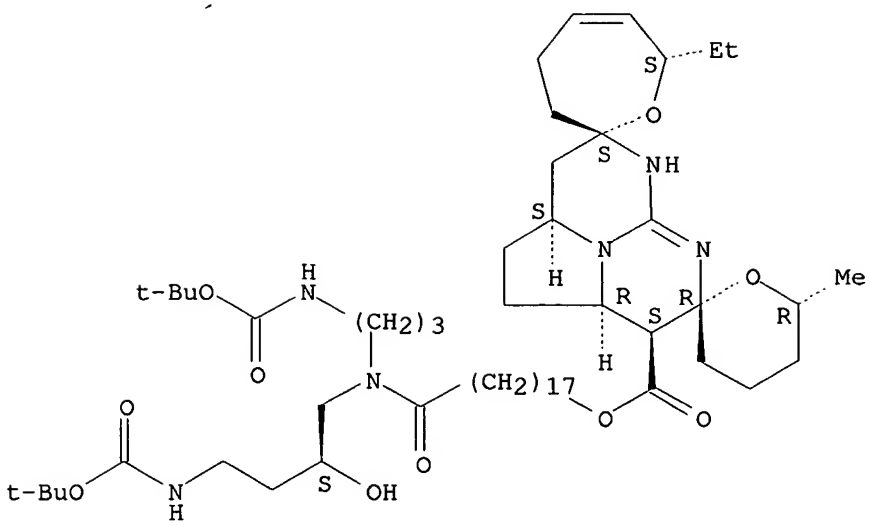
PAGE 2-A

● HCl

RN 600707-08-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 18-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-18-oxooctadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

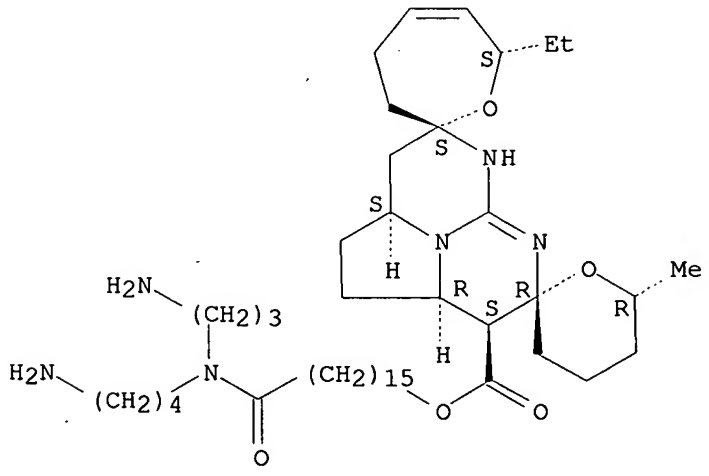


PAGE 2-A

● HCl

L11 ANSWER 14 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:561403 CAPLUS
DN 139:350870
TI Stereoselective synthesis of novel ptilomycalin a analogs via successive 1,3-dipolar cycloaddition reactions and their Ca2+-ATPase inhibitory activity
AU Georgieva, Angelina; Hirai, Manabu; Hashimoto, Yuichi; Nakata, Tadashi; Ohizumi, Yasushi; Nagasawa, Kazuo
CS Institute of Physical and Chemical Research (RIKEN), Saitama, 351-0198, Japan
SO Synthesis (2003), (9), 1427-1432
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 139:350870
AB The pentacyclic guanidine compds. I and II (R = H, R1) were stereoselectively synthesized as novel ptilomycalin A and crambescidin analogs. The synthetic method involves successive 1,3-dipolar cycloaddn. reactions which effectively access the key intermediates, trans- and cis-2,5-disubstituted pyrrolidine having hydroxyl groups at the β-positions on their side chains. Among the analogs synthesized, I and II (R = R1) exhibited significant inhibitory activity against Ca2+-ATPase.
IT 124512-47-6DP, Ptilomycalin a, analogs
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective synthesis of novel ptilomycalin a analogs via successive 1,3-dipolar cycloaddn. reactions and their Ca2+-ATPase inhibitory activity)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

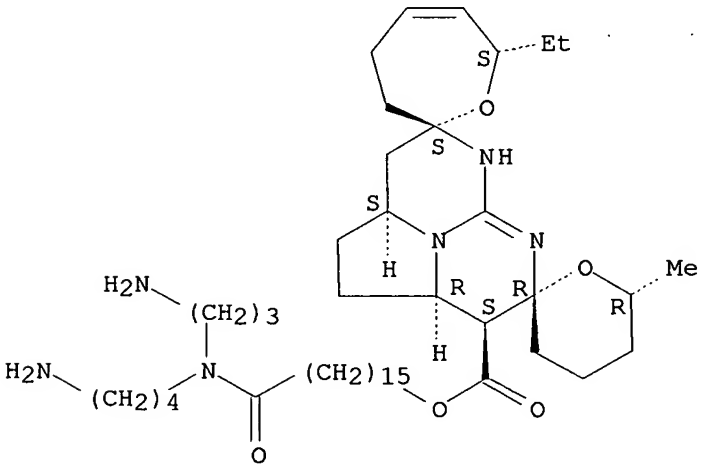
Absolute stereochemistry. Rotation (-).



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD

L11 ANSWER 15 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:943486 CAPLUS
DN 138:304432
TI A synthesis of crambescidin 359
AU Moore, Christopher G.; Murphy, Patrick J.; Williams, Harri L.; McGown, Alan T.; Smith, Nigel K.
CS Department of Chemistry, University of Wales, Bangor, Gwynedd, LL57 2UW, UK
SO Tetrahedron Letters (2002), Volume Date 2003, 44(2), 251-254
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 138:304432
AB A potentially biomimetic synthesis of the guanidine-containing marine natural product crambescidin 359 [I.Cl- (prepared as tetrafluoroborate)] via a double Michael addition of guanidine to a suitably functionalized bis-enone is reported.
IT 124512-47-6, Ptilomycalin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(cytotoxicity against various cancer cell lines)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

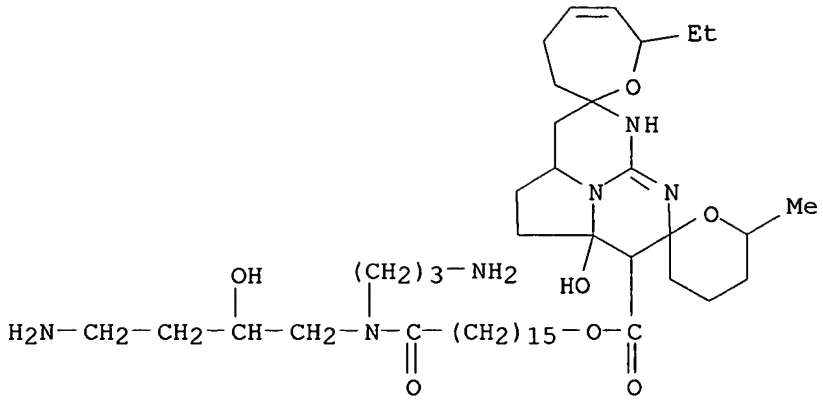


RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 16 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:521462 CAPLUS
DN 137:88442
TI Incensole and furanogermacrens and compounds in treatment for inhibiting neoplastic lesions and microorganisms
IN Shanahan-Pendergast, Elisabeth
PA Ire.
SO PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

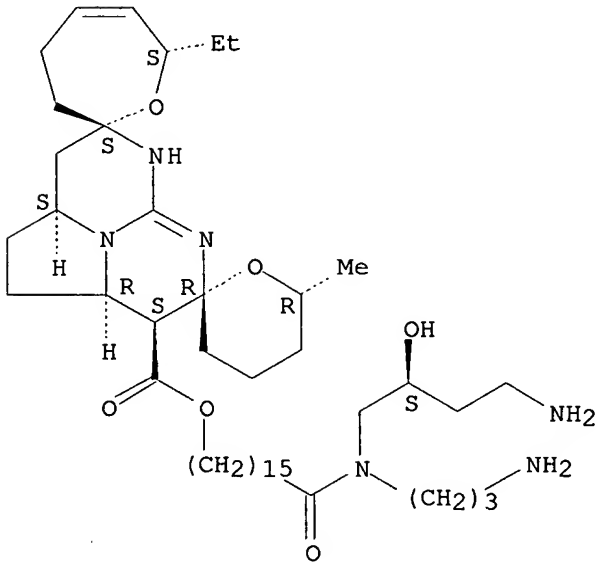
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002053138	A2	20020711	WO 2002-IE1	20020102
	WO 2002053138	A3	20020919		
	W: AE, AG, AT, AU, BB, BG, CA, CH, CN, CO, CU, CZ, LU, LV, MA, MD, UA, UG, US, VN, YU, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, AT, BE, CH, CY, DE, ES, FI, ML, MR, NE, SN, TD, TG				
	AU 2002219472	A1	20020716	AU 2002-219472	20020102
	EP 1351678	A2	20031015	EP 2002-727007	20020102
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2004092583	A1	20040513	US 2004-250535	20040102
PRAI	IE 2001-2	A	20010102		
	WO 2002-IE1	W	20020102		

OS MARPAT 137:88442
AB The invention discloses the use of incensole and/or furanogermacrens, derivs. metabolites and precursors thereof in the treatment of neoplasia, particularly resistant neoplasia and immunodysregulatory disorders. These compds. can be administered alone or in combination with conventional chemotherapeutic, antiviral, antiparasite agents, radiation and/or surgery. Incensole and furanogermacren and their mixture showed antitumor activity against various human carcinomas and melanomas and antimicrobial activity against Staphylococcus aureus and Enterococcus faecalis.
IT 135257-45-3, Crambescidin 816
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical formulation further including; incensole and furanogermacrens and compds. as antitumor and antimicrobial agents)
RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



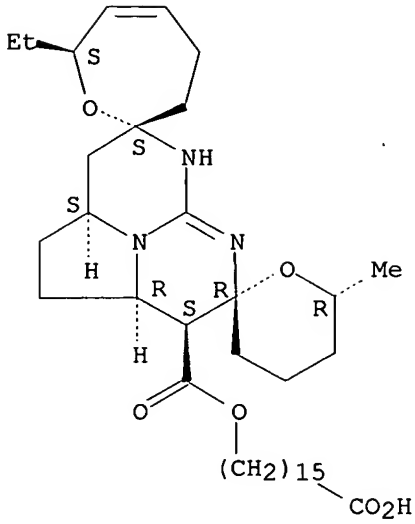
L11 ANSWER 17 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:304407 CAPLUS
DN 136:151335
TI The tethered Biginelli condensation and the enantioselective synthesis of crambescidin 800, crambescidin 657 and neofolitispate 2 and progress towards the total synthesis of asparagamine A and stemofoline
AU McDonald, Andrew Ian
CS Univ. of California, Irvine, CA, USA
SO (2000) 160 pp. Avail.: UMI, Order No. DA9974156
From: Diss. Abstr. Int., B 2000, 61(5), 2541
DT Dissertation
LA English
AB Unavailable
IT 135257-46-4P, Crambescidin 800 214215-58-4P, Crambescidin 657 229160-51-4P, Neofolitispate 2
RL: SPN (Synthetic preparation); PREP (Preparation)
(tethered Biginelli condensation and enantioselective synthesis of crambescidin 800, crambescidin 657 and neofolitispate 2 and progress towards total synthesis of asparagamine A and stemofoline)
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



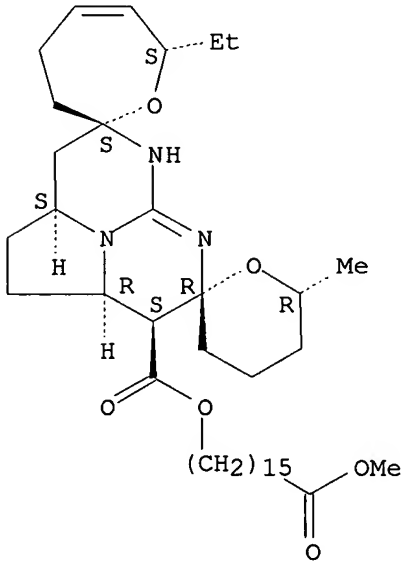
RN 214215-58-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



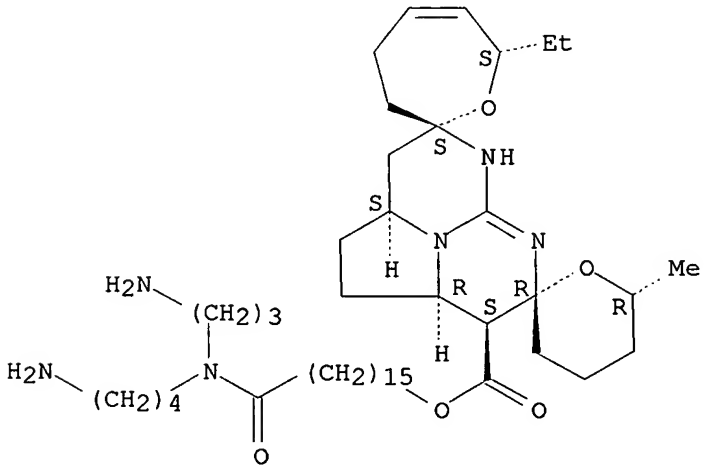
RN 229160-51-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-methoxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L11 ANSWER 18 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:292810 CAPLUS
DN 135:92768
TI Synthesis and biological activity of analogues of ptilomycalin A
AU Black, G. P.; Coles, S. J.; Hizi, A.; Howard-Jones, A. G.; Hursthouse, M. B.; McGown, A. T.; Loya, S.; Moore, C. G.; Murphy, P. J.; Smith, N. K.; Walshe, N. D. A.
CS Department of Chemistry, University of Wales, Gwynedd, Bangor, LL57 2UW, UK
SO Tetrahedron Letters (2001), 42(19), 3377-3381
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 135:92768
AB Benzo-fused model compds. I (X = CH2, n = 12; X = O; n = 10), resembling in structure the marine metabolite ptilomycalin A, were prepared and were shown to display significant activity against a series of cancer cell lines and to also possess a significant activity against the DNA polymerase activity of the reverse transcriptase of human immunodeficiency virus type 1 (HIV-1 RT).
IT 124512-47-6, Ptilomycalin A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(cytotoxic activity and HIV-1 reverse transcriptase inhibitory activity of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 19 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:12459 CAPLUS
DN 134:86416
TI Preparation of hexahydropyrrolo[1,2-c]pyrimidines, guanidinium alkaloids, as antiviral, antifungal and/or antitumor agents
IN Overman, Larry A.; Stappenbeck, Frank; Mcdonald, Andrew I.
PA The Regents of the University of California, USA
SO PCT Int. Appl., 222 pp.
CODEN: PIXXD2
DT Patent
LA English

Appl PCT

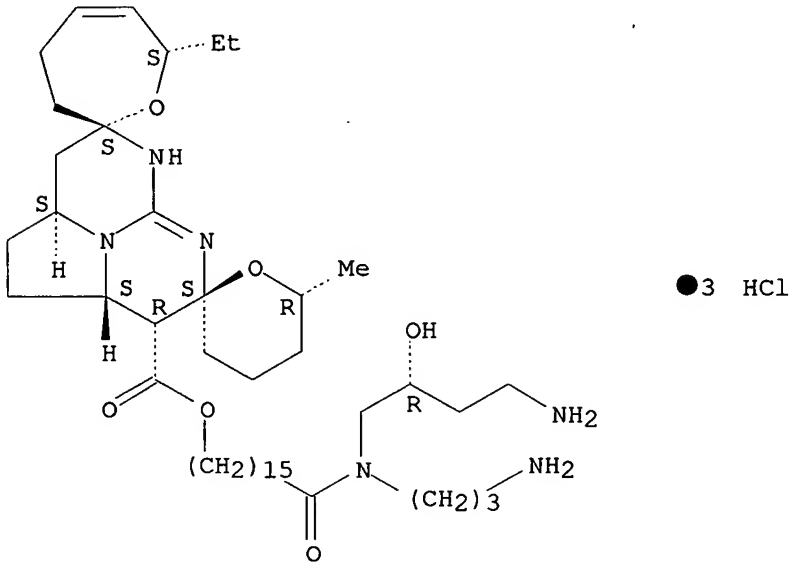
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001000626	A1	20010104	WO 2000-US18395	20000630
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2376758	AA	20010104	CA 2000-2376758	20000630
	EP 1204666	A1	20020515	EP 2000-947033	20000630
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003503411	T2	20030128	JP 2001-507034	20000630
	BR 2000011912	A	20030624	BR 2000-11912	20000630
	NZ 516917	A	20030926	NZ 2000-516917	20000630
	AU 777578	B2	20041021	AU 2000-60703	20000630
	ZA 2001010327	A	20030314	ZA 2001-10327	20011214
	US 2003176697	A1	20030918	US 2002-255994 Pending	20020924
	US 2005239804	A1	20051027	US 2004-815023	20040330
	AU 2004231239	A1	20041223	AU 2004-231239	20041119
PRAI	US 1999-142027P	P	19990630		
	US 1999-142028P	P	19990630		
	WO 2000-US18395	W	20000630		
	US 2001-18630	A2	20011214		

OS MARPAT 134:86416
AB Antiviral, antifungal and/or antitumor agents, hexahydropyrrolo[1,2-c]pyrimidines, guanidinium alkaloids, I (R = H, carboxylic acid protecting group, an ω-alkoxycarboxylic acid or ester; X = any pharmaceutically acceptable counterion) were prepared In vitro screening of 60 tumor cell lines against pharmaceutical compns. I to determine antitumor activity is described. Enantioselective synthesis of guanidinium alkaloid compds. with cis- or trans-1-oxo- and -1-iminohexahydropyrrolo[1,2-c]pyrimidine units including, 13,14,15-isocrambescidin 800, crambescidin 800 and ptilomycalin A was accomplished. Methods for preparing novel pentacyclic intermediates for the preparation of the crambescidin/ptilomycalin family of guanidinium alkaloids and congeners are also disclosed.
IT 276878-01-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of hexahydropyrrolo[1,2-c]pyrimidines as antiviral, antifungal and/or antitumor agents)

RN 276878-01-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2R)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

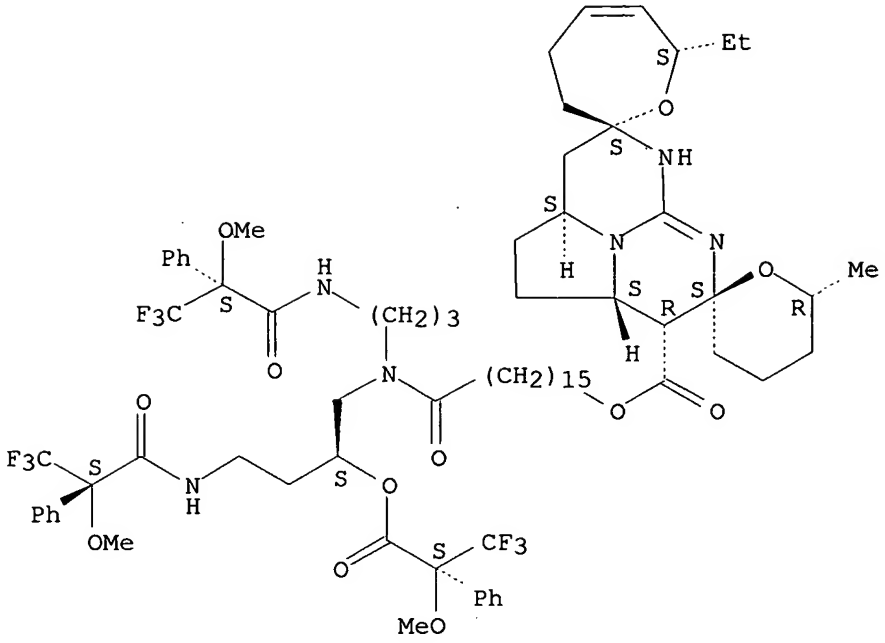
Absolute stereochemistry.



IT 316831-10-4P 316831-11-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hexahydropyrrolo[1,2-c]pyrimidines as antiviral, antifungal and/or antitumor agents)
RN 316831-10-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2S)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

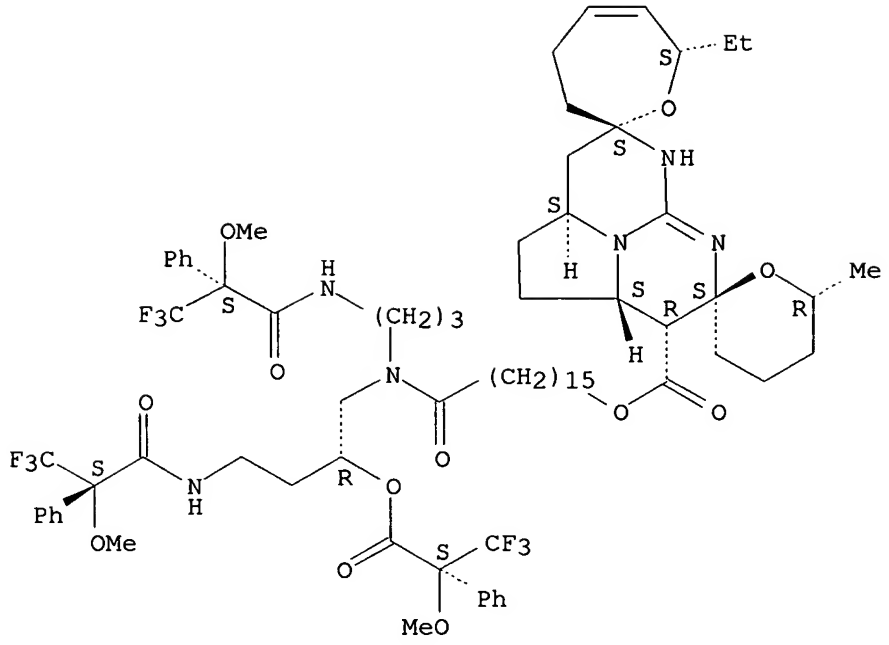
● HCl

RN 316831-11-5 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2R)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

● HCl

IT 162145-92-8P 162240-64-4P 246266-20-6P
246266-22-8P 246516-57-4P 246851-97-8P,
13,14,15-Isocrambescidin 800 trihydrochloride 275808-01-0P,
(-)-Ptilomycalin A trihydrochloride 275808-03-2P, Crambescidin
800 trihydrochloride 275808-29-2P 275808-55-4P
275808-56-5P 275808-57-6P 275823-78-4P
276877-93-1P 316830-89-4P 316831-29-5P
316831-34-2P 317831-96-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of hexahydropyrrolo[1,2-c]pyrimidines as antiviral, antifungal and/or antitumor agents)

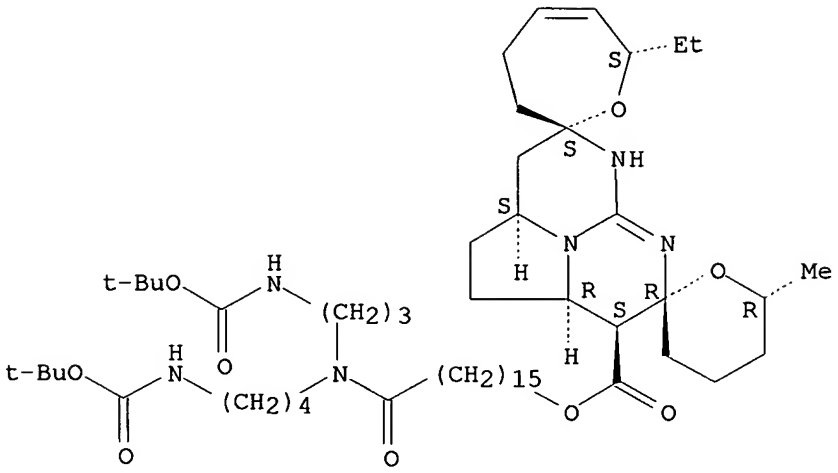
RN 162145-92-8 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

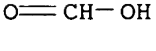
CRN 162145-91-7
CMF C55 H96 N6 O9

Absolute stereochemistry. Rotation (-).



CM 2

CRN 64-18-6
CMF C H2 O2

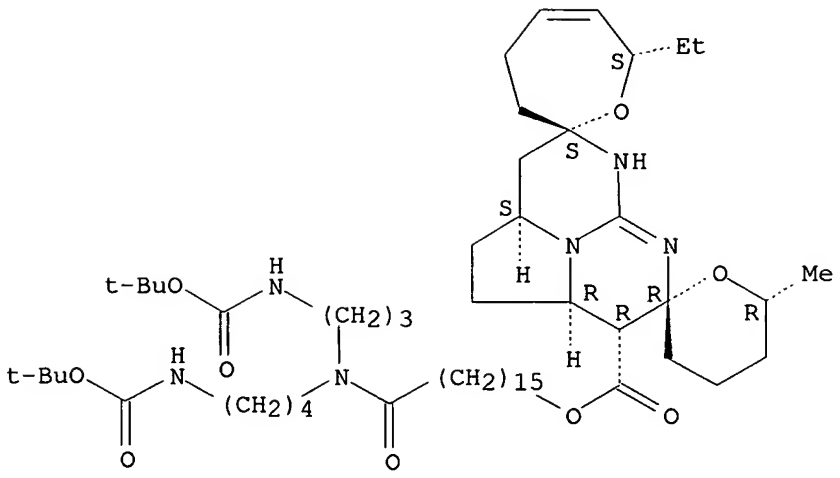


RN 162240-64-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

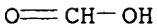
CRN 162240-63-3
CMF C55 H96 N6 O9

Absolute stereochemistry. Rotation (+).



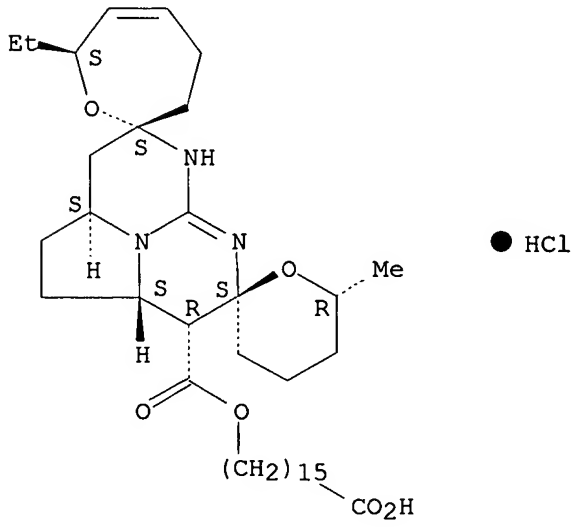
CM 2

CRN 64-18-6
CMF C H2 O2



RN 246266-20-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 246266-22-8 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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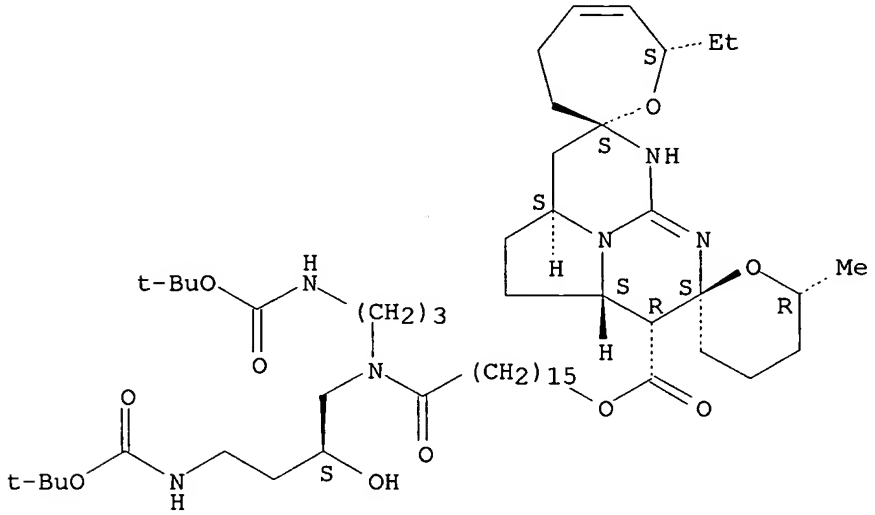


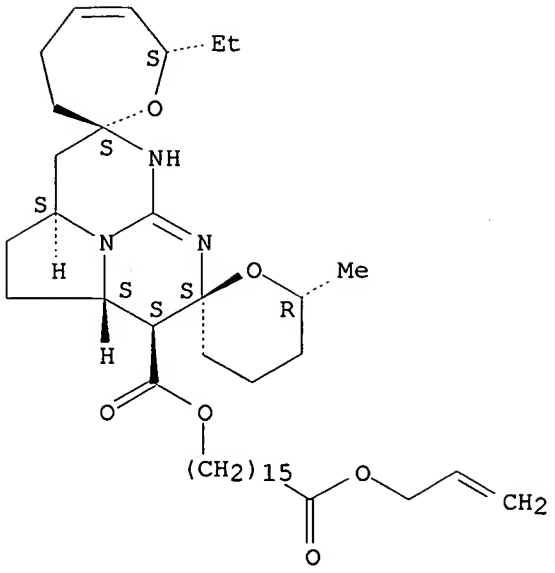
PAGE 2-A

● HCl

RN 246516-57-4 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

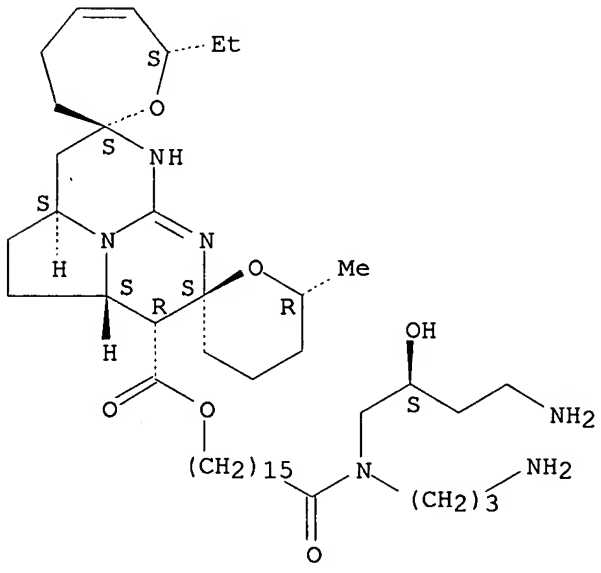
Absolute stereochemistry. Rotation (-).



● HCl

RN 246851-97-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

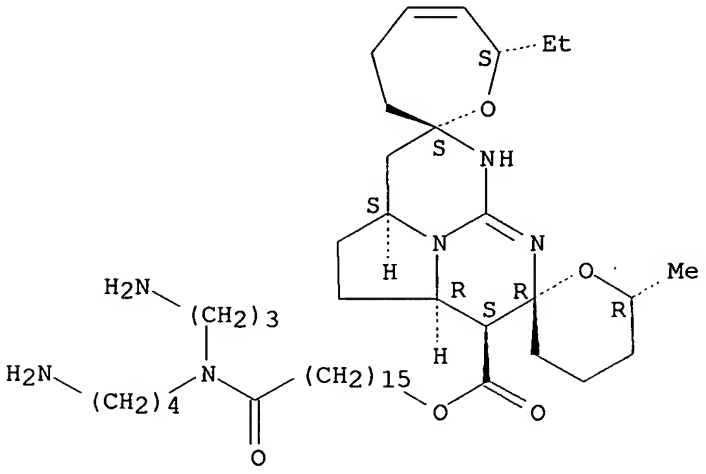


●3 HCl

RN 275808-01-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-

oxohexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

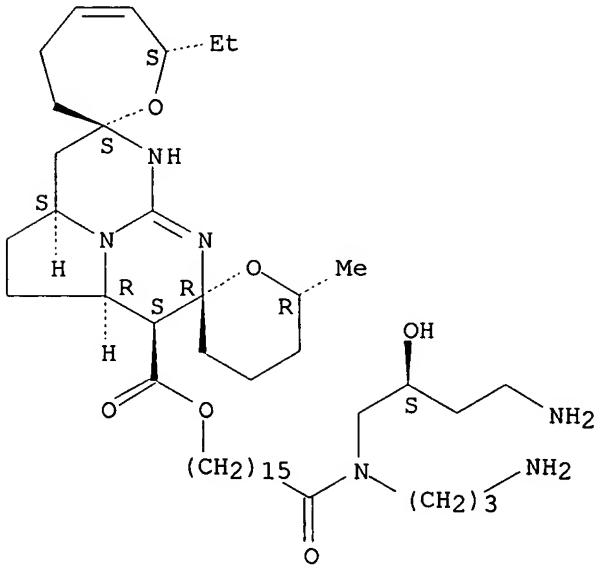


●3 HCl

RN 275808-03-2 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



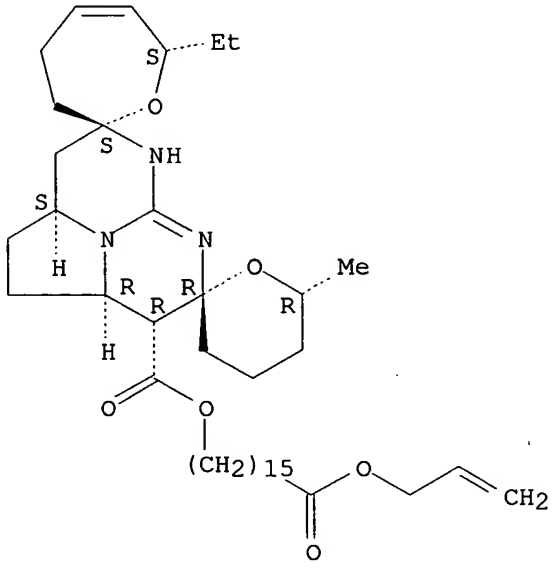
●3 HCl

RN 275808-29-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

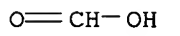
CRN 275808-28-1
CMF C41 H67 N3 O6

Absolute stereochemistry. Rotation (+).



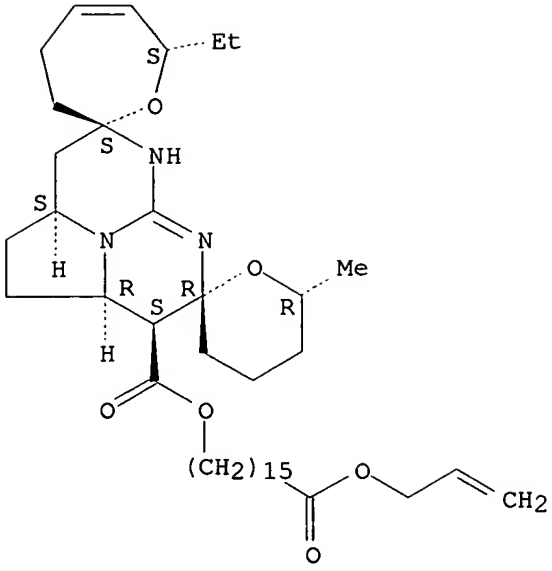
CM 2

CRN 64-18-6
CMF C H2 O2



RN 275808-55-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● HCl

RN 275808-56-5 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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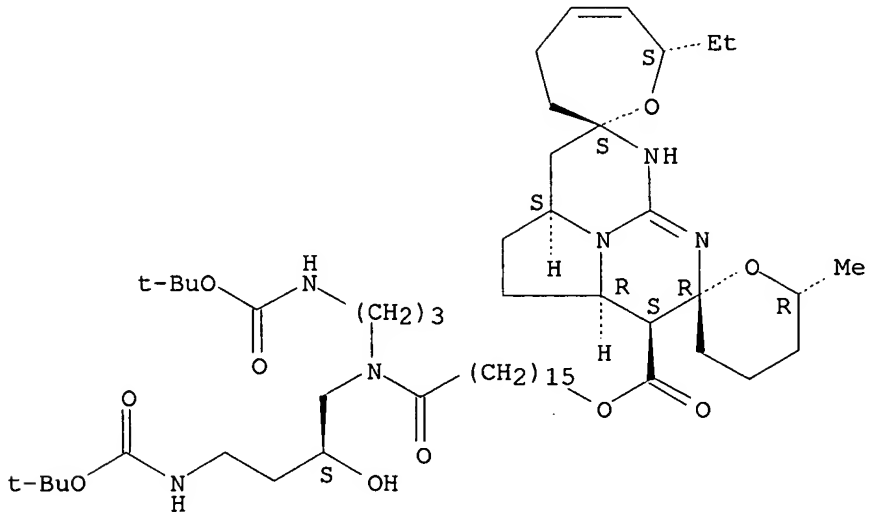

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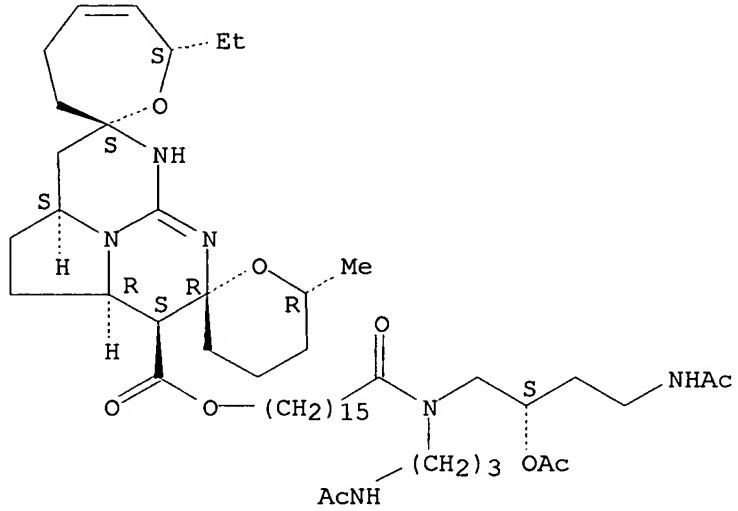
● HCl

RN 275808-57-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

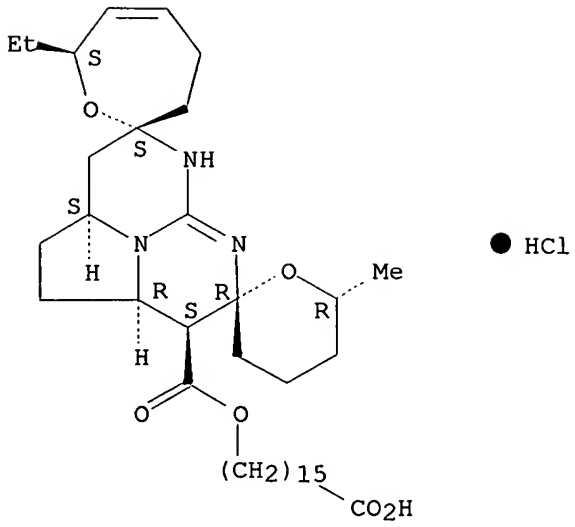


PAGE 2-A

● HCl

RN 275823-78-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

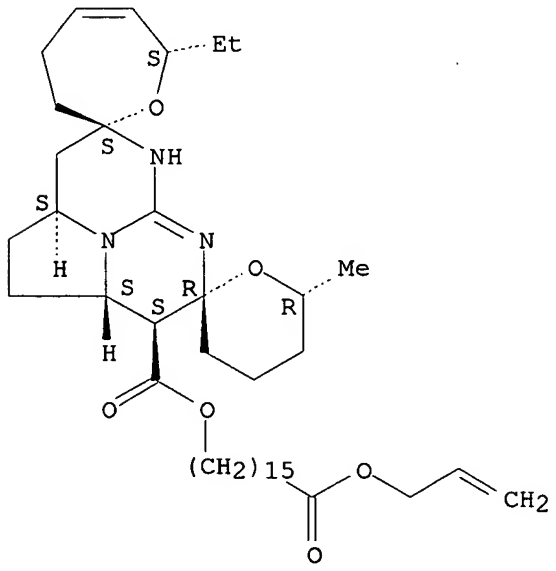


RN 276877-93-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)-, monoformate (9CI) (CA INDEX NAME)

CM 1

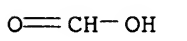
CRN 276877-92-0
CMF C41 H67 N3 O6

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

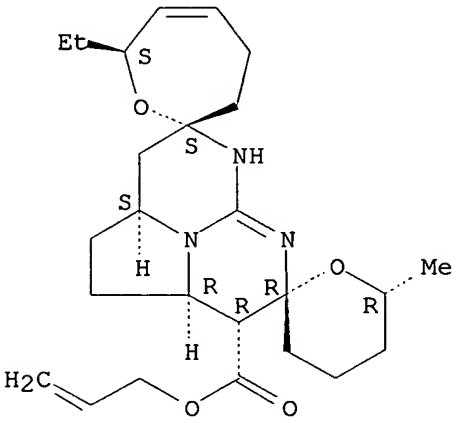


RN 316830-89-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 2-propenyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 316830-88-3
CMF C25 H37 N3 O4

Absolute stereochemistry.

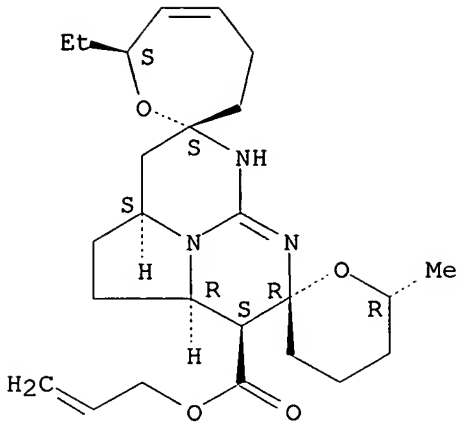


CM 2

CRN 64-18-6
CMF C H2 O2

RN 316831-29-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 2-propenyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

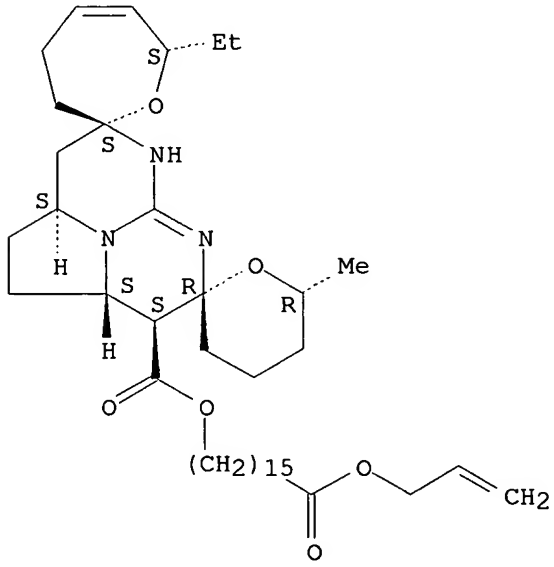
Absolute stereochemistry.



● HCl

RN 316831-34-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



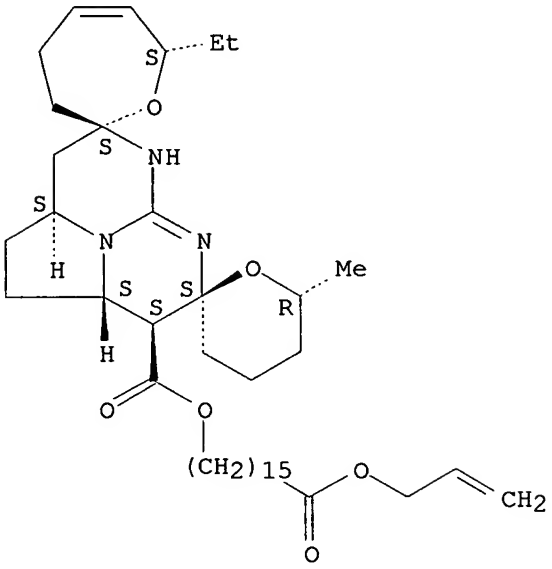
● HCl

RN 317831-96-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)-, monoformate (9CI) (CA INDEX NAME)

CM 1

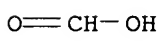
CRN 317831-95-1
CMF C41 H67 N3 O6

Absolute stereochemistry. Rotation (-).



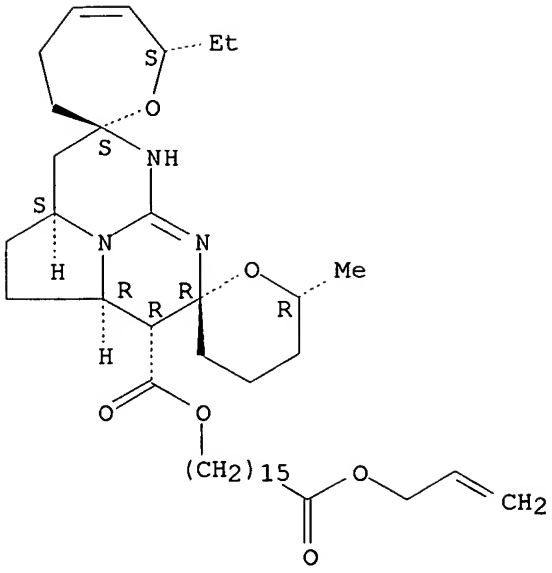
CM 2

CRN 64-18-6
CMF C H2 O2



IT 275808-54-3 317831-94-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(preparation of hexahydropyrrolo[1,2-c]pyrimidines as antiviral, antifungal and/or antitumor agents)
RN 275808-54-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



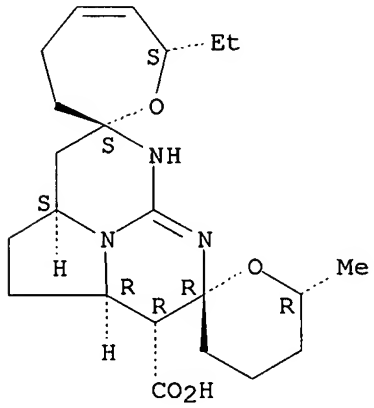
● HCl

RN 317831-94-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 317831-93-9
CMF C22 H33 N3 O4

Absolute stereochemistry.



CM 2

CRN 64-18-6
CMF C H2 O2

O═CH—OH

IT 125422-23-3P 214215-60-8P 246266-23-9P
276878-95-6P 316831-04-6P 317831-97-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hexahydropyrrolo[1,2-c]pyrimidines as antiviral, antifungal and/or antitumor agents)

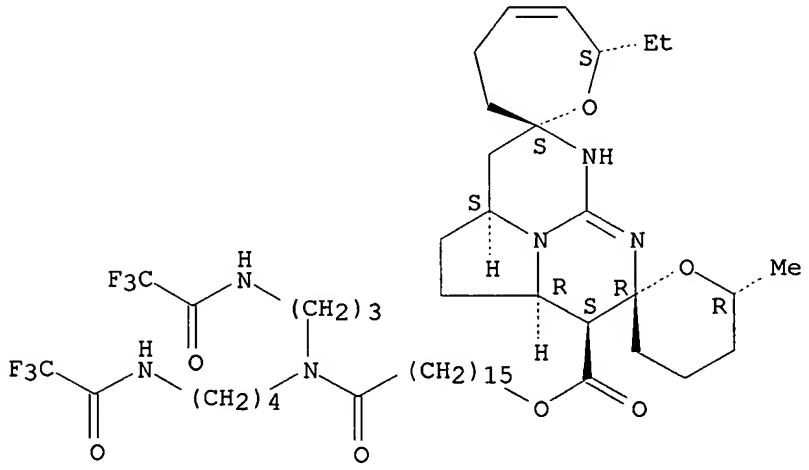
RN 125422-23-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[4-[(trifluoroacetyl)amino]butyl][3-[(trifluoroacetyl)amino]propyl]amino]hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

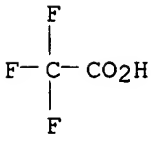
CRN 125422-22-2
CMF C49 H78 F6 N6 O7

Absolute stereochemistry. Rotation (-).



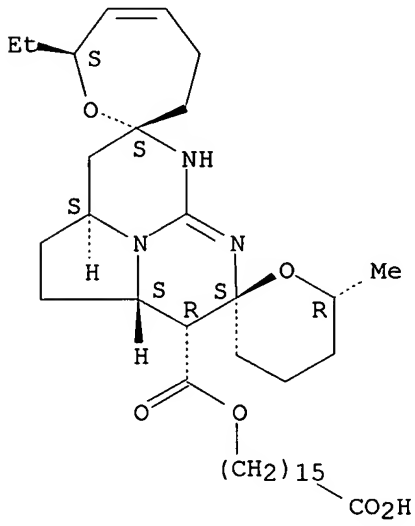
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 214215-60-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

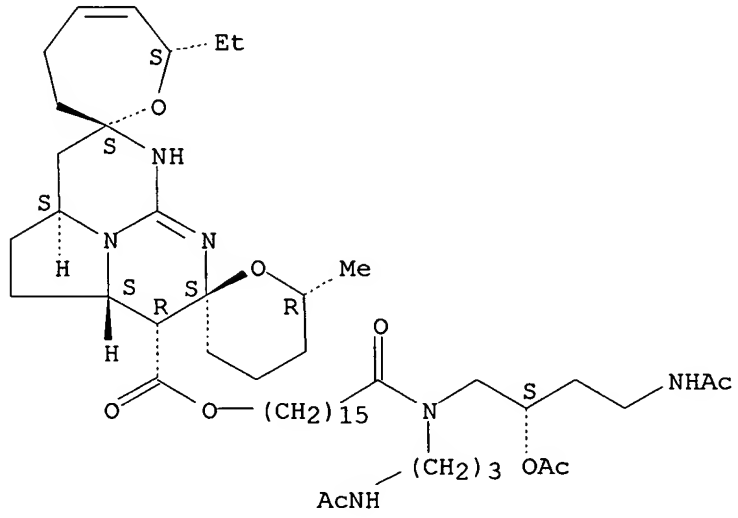
Absolute stereochemistry. Rotation (-).



RN 246266-23-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

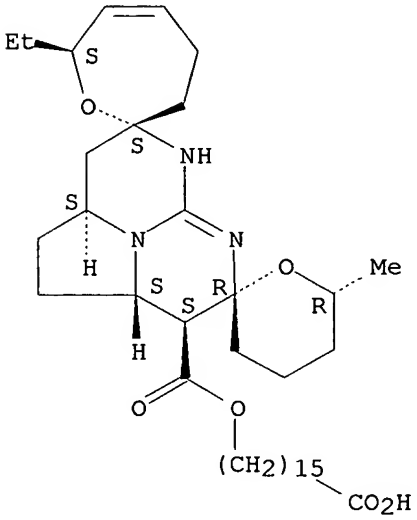


PAGE 2-A

● HCl

RN 276878-95-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

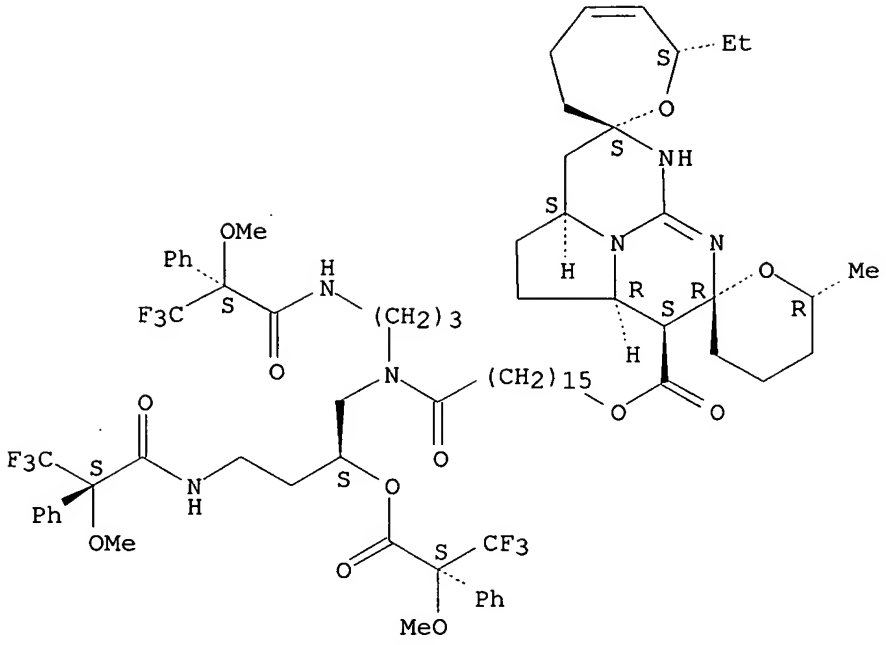


● HCl

RN 316831-04-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2S)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

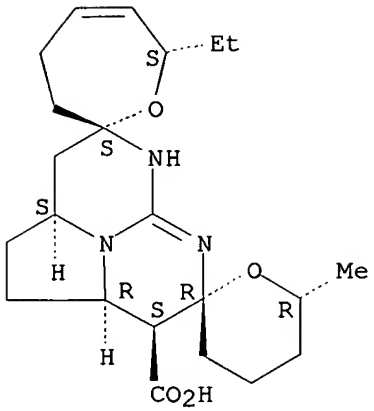


PAGE 2-A

●3 HCl

RN 317831-97-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



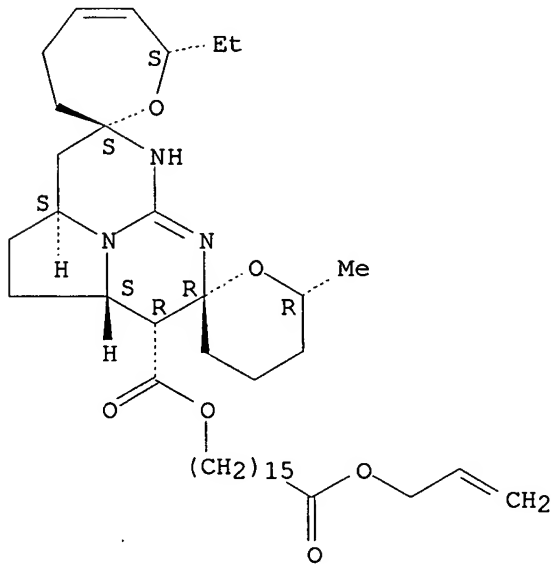
● HCl

IT 276878-06-9P 316831-35-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hexahydropyrrolo[1,2-c]pyrimidines as antiviral, antifungal and/or antitumor agents)

RN 276878-06-9 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



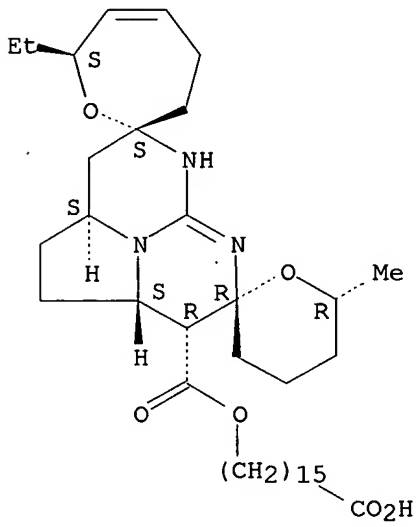
● HCl

RN 316831-35-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8'

,8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

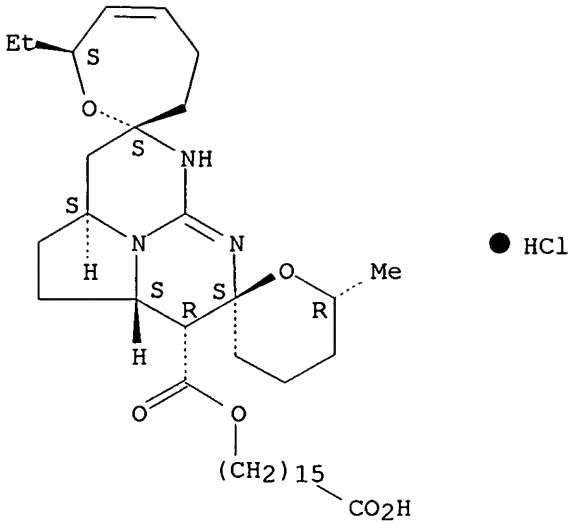
Absolute stereochemistry.



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

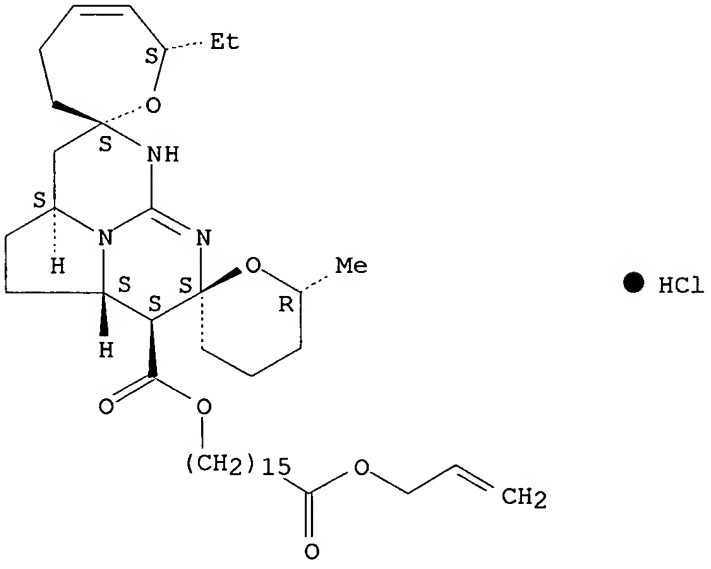
L11 ANSWER 20 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:293396 CAPLUS
DN 133:58969
TI Enantioselective Total Syntheses of 13,14,15-Isocrambescidin 800 and 13,14,15-Isocrambescidin 657
AU Coffey, D. Scott; Overman, Larry E.; Stappenbeck, Frank
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Journal of the American Chemical Society (2000), 122(20), 4904-4914
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 133:58969
AB The first total syntheses of 13,14,15-isocrambescidin 800 [I·Cl-; R = NH(CH2CH2CH2NH2)CH2CH(OH)CH2CH2NH2-(S)] and 13,14,15-isocrambescidin 657 (I; R = O-) were accomplished in convergent fashion. The central strategic step was a tethered Biginelli condensation of guanidine aminal II·HCl [TIPS = Si(CHMe2)3] and β-ketoester, (R)-H2C:CHCH2O2C(CH2)15O2CCH2C(:O)(CH2)3CHMeOSiMe2CMe3, to give 1-iminohexahydropyrrolo[1,2-c]pyrimidine carboxylic ester III·HCl [R1 = (CH2)15CO2CH2CH:CH2, R2 = TBDMS, R3 = TIPS; TBDMS = SiMe2CMe3]. This step united all the heavy atoms of the pentacyclic guanidine nucleus and set the critical trans C10-C13 stereorelationship. Acidic treatment of derivative III·HCl [R1 = (CH2)15CO2CH2CH:CH2; R2 = R3 = H] triggered tricyclization to generate pentacyclic guanidine IV·Cl- in high yield. After cleavage of the allyl ester, the derived acid underwent coordinated epimerization at C14 and C15 in the presence of triethylamine to form the pentacyclic isocrambescidin nucleus. The synthesis of I was achieved in 11% overall yield from amine V by a sequence involving five isolated intermediates. As detailed in the preceding account, V can be accessed from com. available 3-butyn-1-ol in 30% overall yield by way of nine isolated and purified intermediates. Mosher derivs. were prepared from (S)-(-)-α-methoxy-α-(trifluoromethyl)phenylacetic acid and natural I [R = NH(CH2CH2CH2NH2)CH2CH(OH)CH2CH2NH2-(S)], synthetic I [R = NH(CH2CH2CH2NH2)CH2CH(OH)CH2CH2NH2-(S)], and synthetic C43 epimer I·2HCl·Cl- [R = NH(CH2CH2CH2NH2)CH2CH(OH)CH2CH2NH2-(R)]. Anal. by 19F NMR showed that the Mosher derivs. of natural and synthetic I [R = NH(CH2CH2CH2NH2)CH2CH(OH)CH2CH2NH2-(S)]were identical, thus establishing for the first time that the stereochem. of 13,14,15-isocrambescidin 800 [I·Cl-; R = NH(CH2CH2CH2NH2)CH2CH(OH)CH2CH2NH2-(S)] at C43 is S. The mechanism of the tricyclization and epimerization steps is discussed, as are the relative energies of the 13,14,15-isocrambescidin, 13,15-epicrambescidin, and 13-epicrambescidin guanidine moieties.
IT 246266-20-6P 246516-57-4P 276878-06-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total syntheses of isocrambescidin 800 and isocrambescidin 657)
RN 246266-20-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



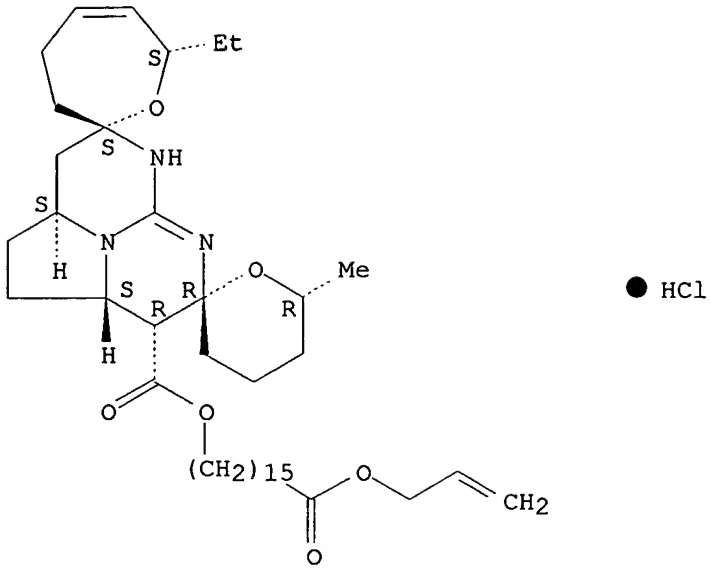
RN 246516-57-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 276878-06-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



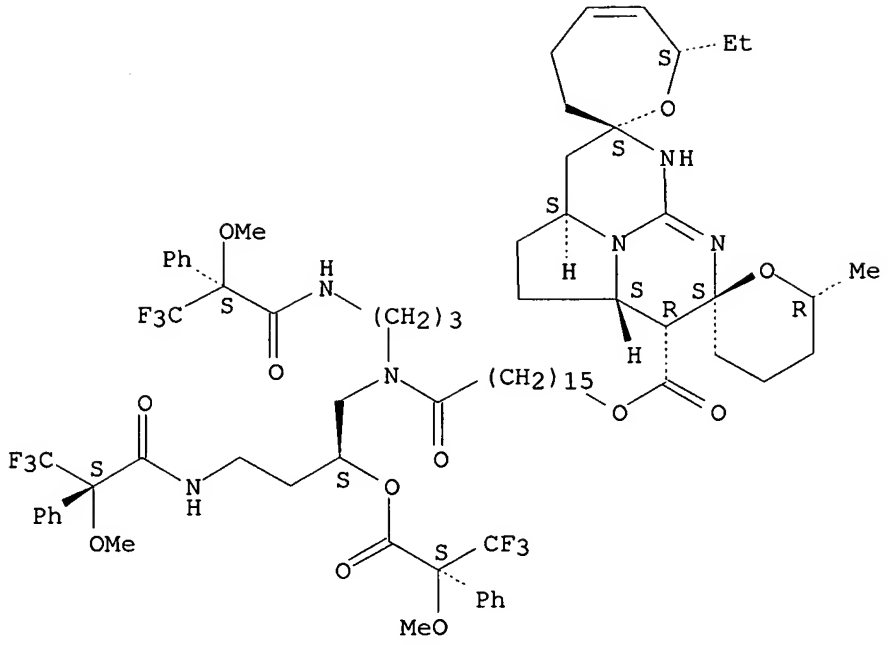
IT 276878-02-5P 276878-03-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total syntheses of isocrambescidin 800 and isocrambescidin 657)

RN 276878-02-5 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2S)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

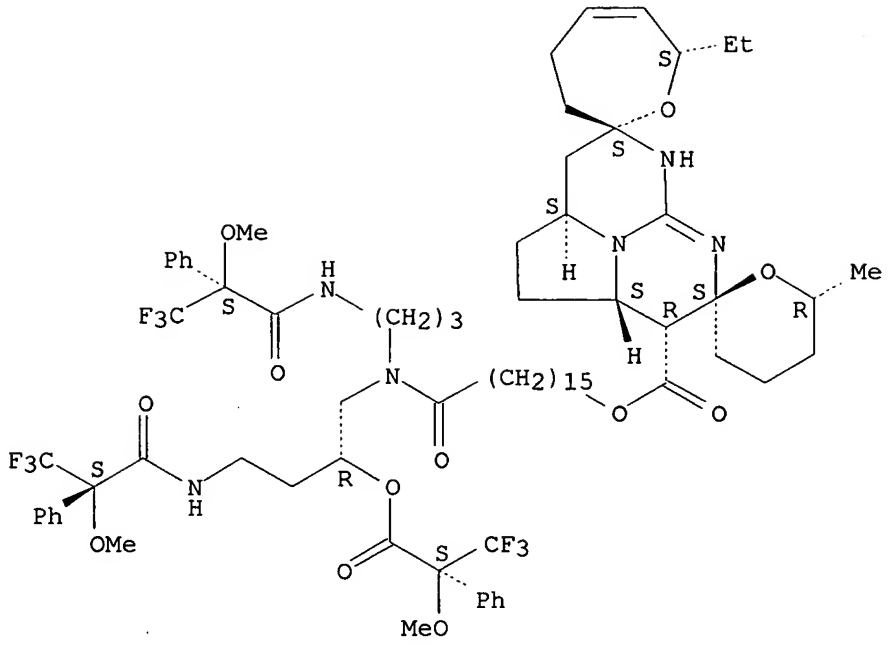
● 3 HCl

RN 276878-03-6 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2R)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

●3 HCl

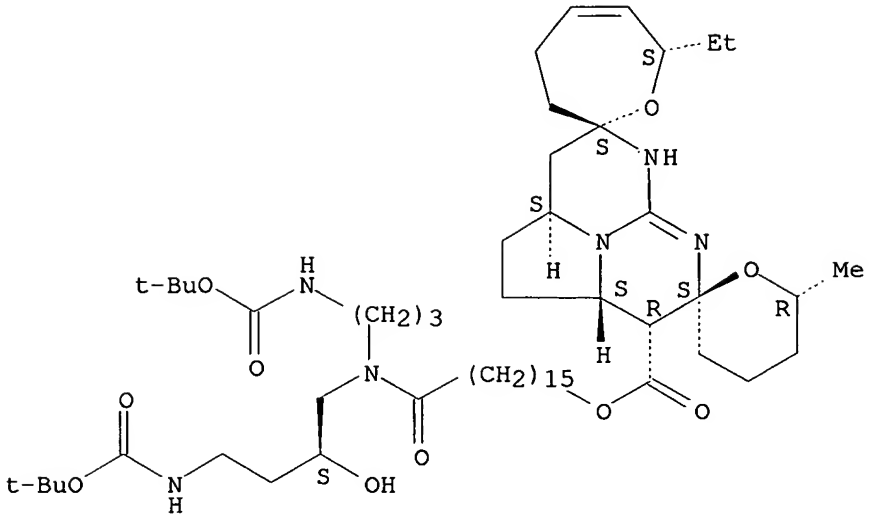
IT 246266-22-8P 246851-97-8P 276877-93-1P
276877-98-6P 276878-01-4P 276878-95-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total syntheses of isocrambescidin 800 and isocrambescidin 657)

RN 246266-22-8 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

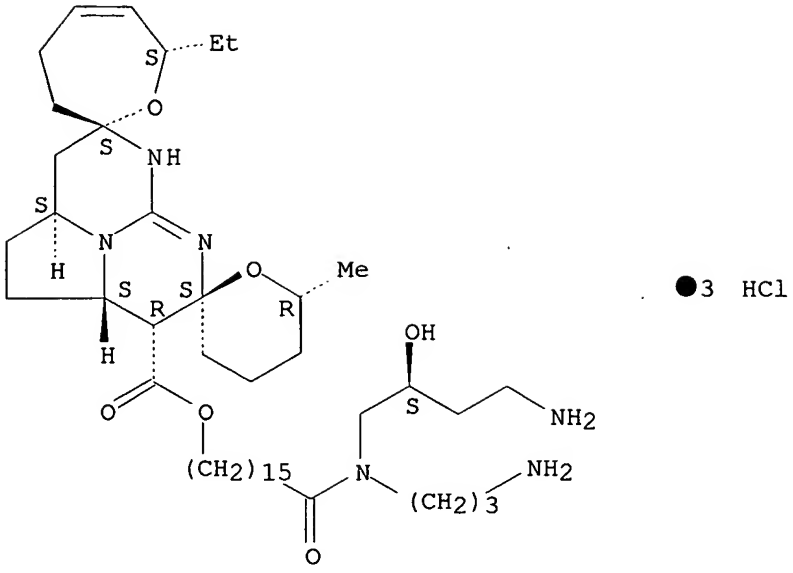


PAGE 2-A

● HCl

RN 246851-97-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



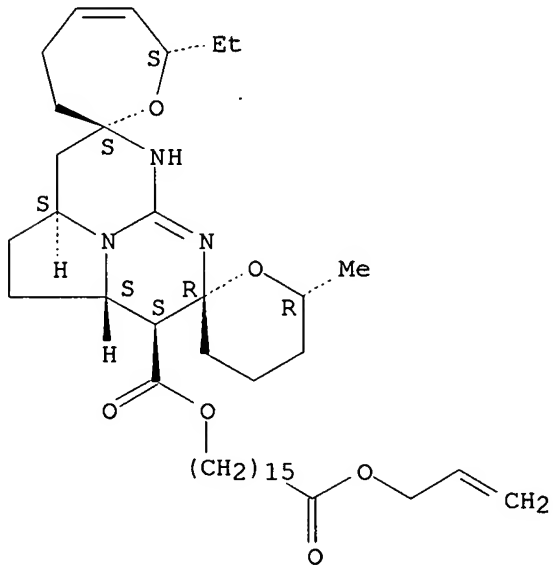
●3 HCl

RN 276877-93-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)-, monoformate (9CI) (CA INDEX NAME)

CM 1

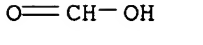
CRN 276877-92-0
CMF C41 H67 N3 O6

Absolute stereochemistry.



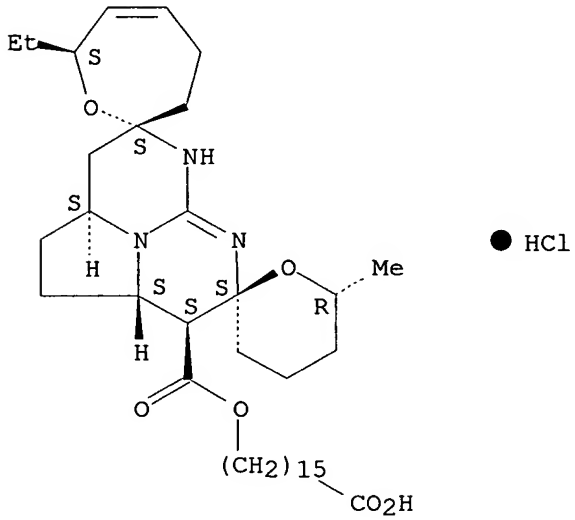
CM 2

CRN 64-18-6
CMF C H2 O2



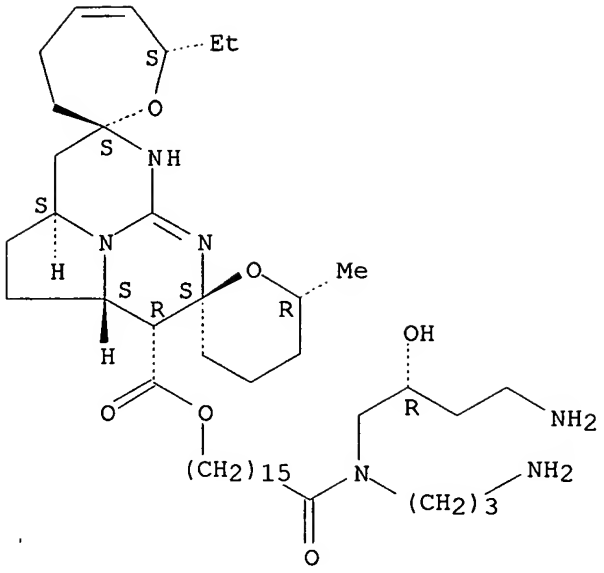
RN 276877-98-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 276878-01-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2R)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

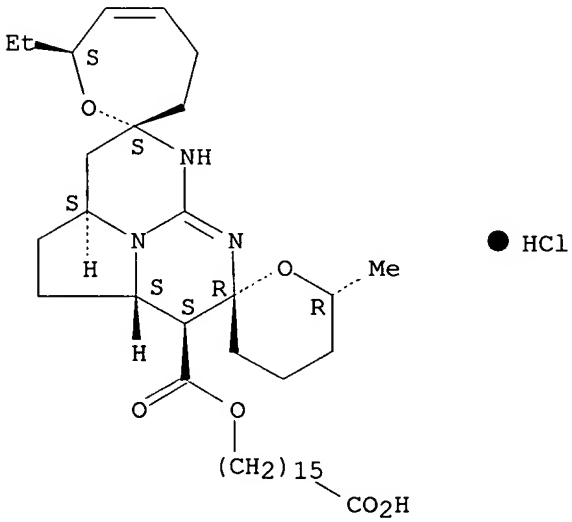
Absolute stereochemistry.



● 3 HCl

RN 276878-95-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

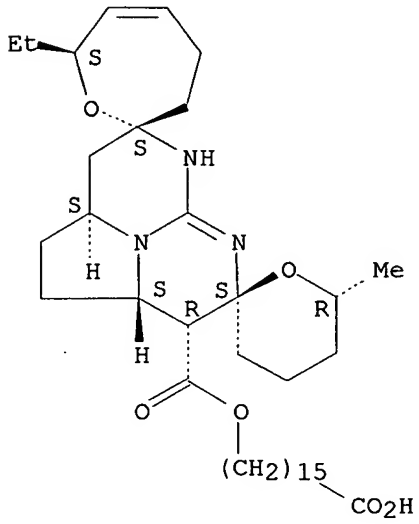


● HCl

IT 214215-60-8P, (-)-13,14,15-Isocrambescidin 657
276878-00-3P 276878-10-5P 276878-14-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total syntheses of isocrambescidin 800 and isocrambescidin 657)
RN 214215-60-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

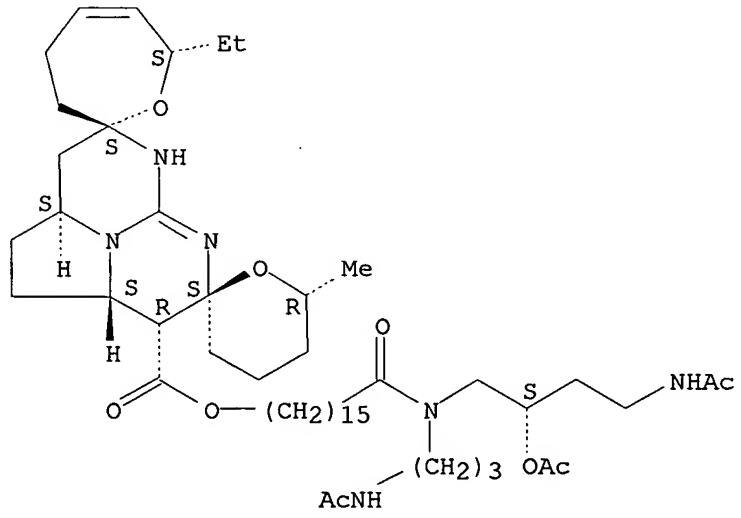


RN 276878-00-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



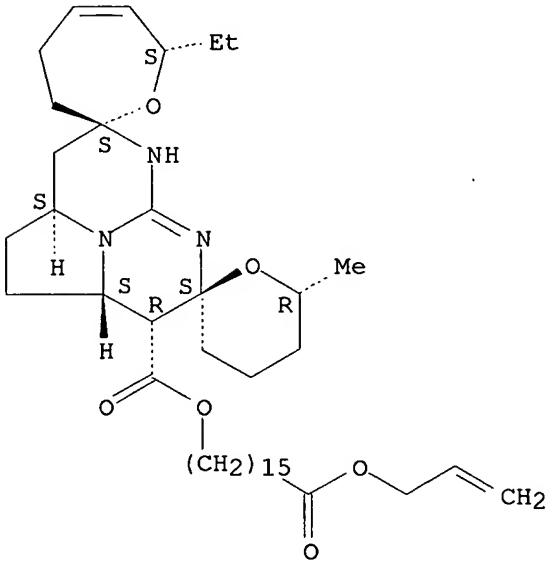
●3 HCl

RN 276878-10-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 276878-09-2
CMF C41 H67 N3 O6

Absolute stereochemistry.



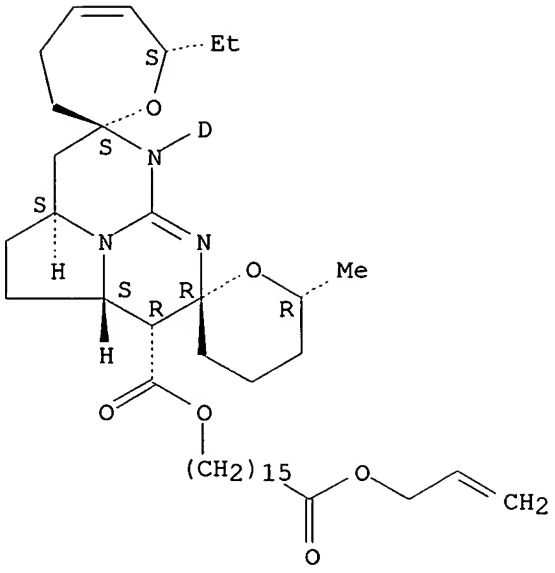
CM 2

CRN 64-18-6
CMF C H2 O2

O═CH—OH

RN 276878-14-9 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, mono(hydrochloride-d), (2S,2''R,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



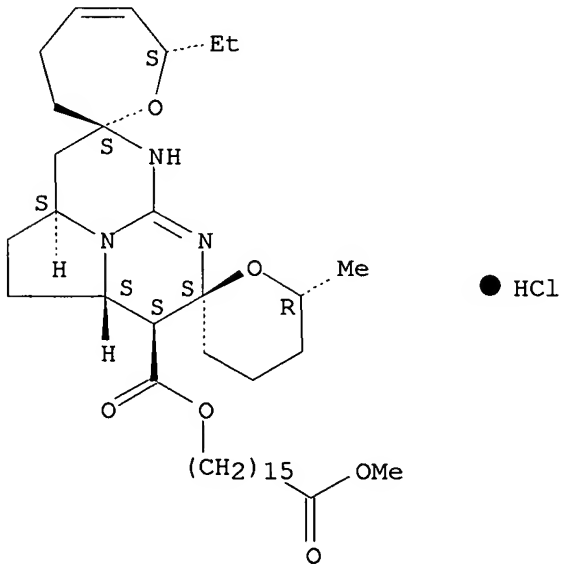
● DCl

IT 276878-13-8 278168-14-2 278168-16-4
278168-65-3 278168-66-4
RL: PRP (Properties)
(mol. modeling; enantioselective total syntheses of isocrambescidin 800 and isocrambescidin 657)

RN 276878-13-8 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-methoxy-16-oxohexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

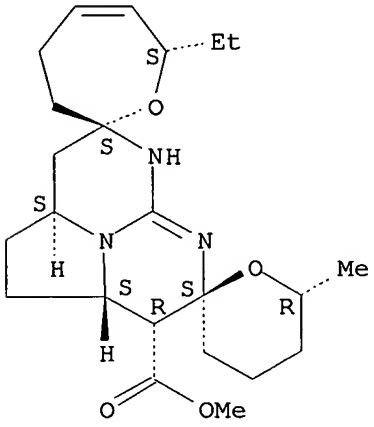
Absolute stereochemistry.



● HCl

RN 278168-14-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, conjugate monoacid, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

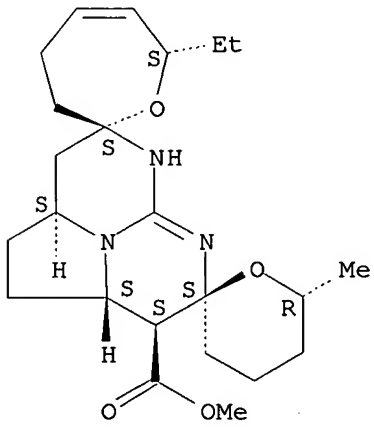
Absolute stereochemistry.



● H^+

RN 278168-16-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, conjugate monoacid, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

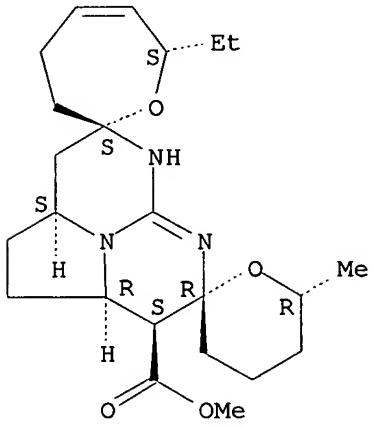
Absolute stereochemistry.



● H^+

RN 278168-65-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, conjugate monoacid, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

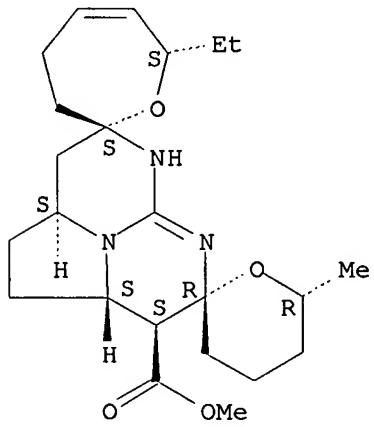
Absolute stereochemistry.



● H^+

RN 278168-66-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, conjugate monoacid, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

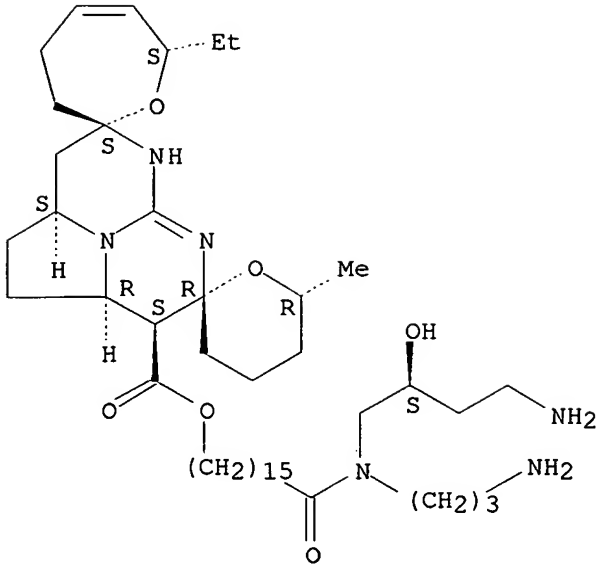


● H^+

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 21 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:293395 CAPLUS
DN 133:43696
TI A Practical Entry to the Crambescidin Family of Guanidine Alkaloids. Enantioselective Total Syntheses of Ptilomycalin A, Crambescidin 657 and Its Methyl Ester (Neofolitispates 2), and Crambescidin 800
AU Coffey, D. Scott; McDonald, Andrew I.; Overman, Larry E.; Rabinowitz, Michael H.; Renhowe, Paul A.
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Journal of the American Chemical Society (2000), 122(20), 4893-4903
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 133:43696
AB Among the most structurally remarkable guanidine natural products are the crambescidin/ptilomycalin A family of marine alkaloids. The evolution of a practical strategy for preparing pharmacol. significant crambescidin/ptilomycalin A alkaloids that lack oxidation at C13 is described. The first total syntheses of crambescidin 800 (2), crambescidin 657 (6), and neofolitispate 2 (7) are reported in full detail. The central strategic step in these convergent total syntheses is tethered Biginelli condensation of a β-keto ester with an ureido aminal to combine all carbons of the guanidine nucleus and set the pivotal C10-C13 stereo-relationship. The total synthesis of crambescidin 800 was accomplished in 3% overall yield from com. available 3-butyn-1-ol by way of 16 isolated and purified intermediates. Full details of our earlier total synthesis of ptilomycalin A (1) are also presented. The total syntheses described in this disclosure confirm the stereochem. assignments of 1, 2, 6, and 7 and rigorously establish that the absolute configuration of the hydroxyspermidine side chain of crambescidin 800 is S.
IT 275808-03-2P, Crambescidin 800 trihydrochloride
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(absolute configuration; enantioselective total synthesis of crambescidin 657, neofolitispate 2, and crambescidin 800)
RN 275808-03-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



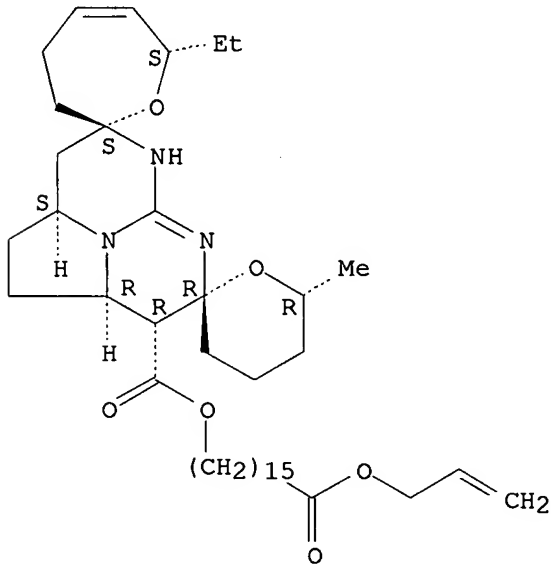
● 3 HCl

IT 275808-54-3P 275808-55-4P 275808-56-5P
275823-78-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total synthesis of crambescidin 657, neofolitispate 2, and crambescidin 800)

RN 275808-54-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)- (9CI) (CA INDEX NAME)

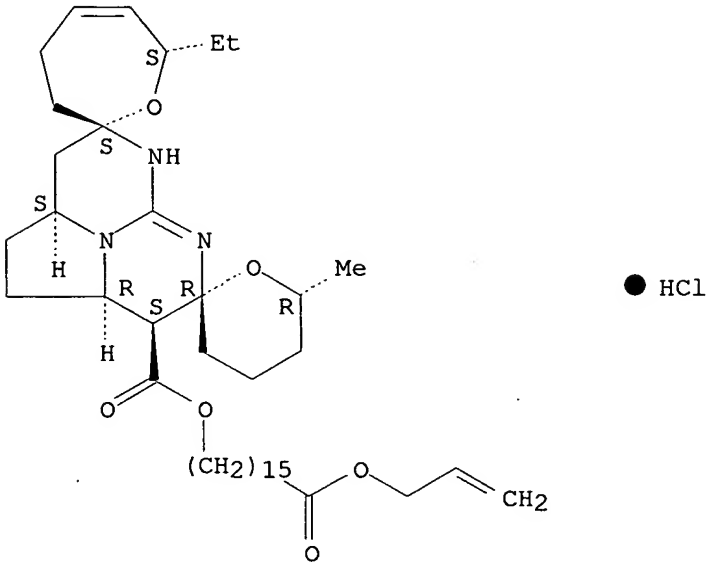
Absolute stereochemistry. Rotation (+).



● HCl

RN 275808-55-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

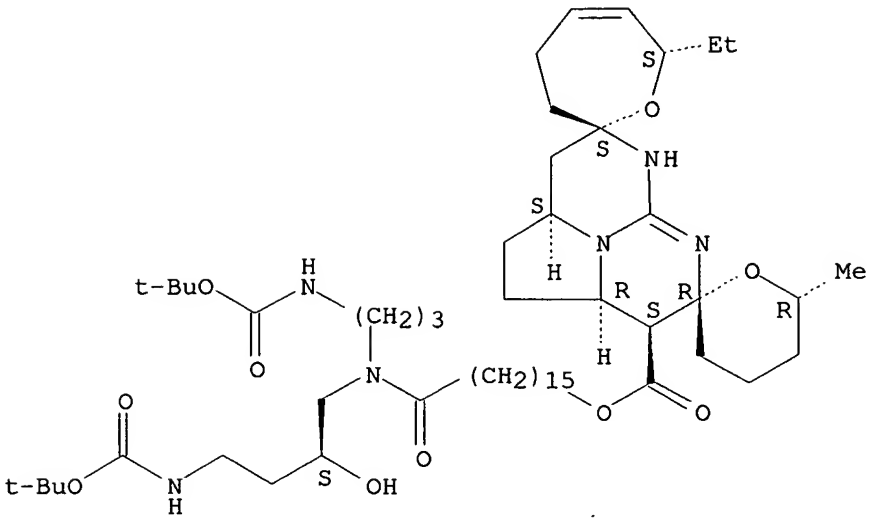
Absolute stereochemistry. Rotation (-).



RN 275808-56-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

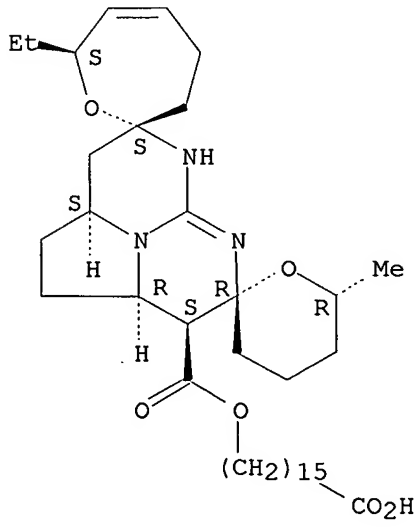


PAGE 2-A

● HCl

RN 275823-78-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



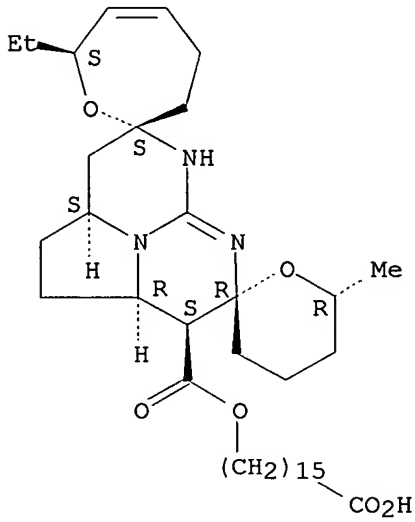
● HCl

IT 214215-58-4P, Crambescidin 657 229160-51-4P,

Neofolitispate 2 275808-57-6P 275808-58-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total synthesis of crambescidin 657, neofolitispate 2, and crambescidin 800)

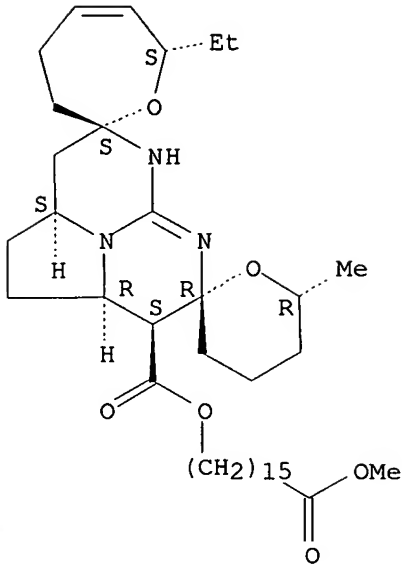
RN 214215-58-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 229160-51-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-methoxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

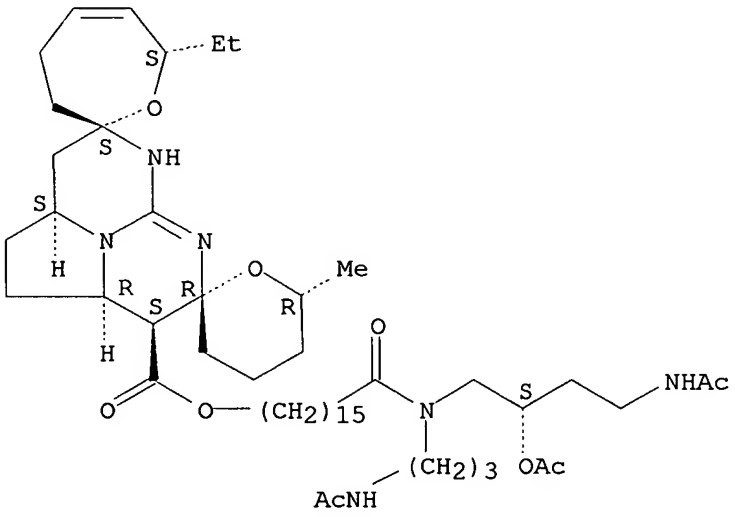


RN 275808-57-6 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



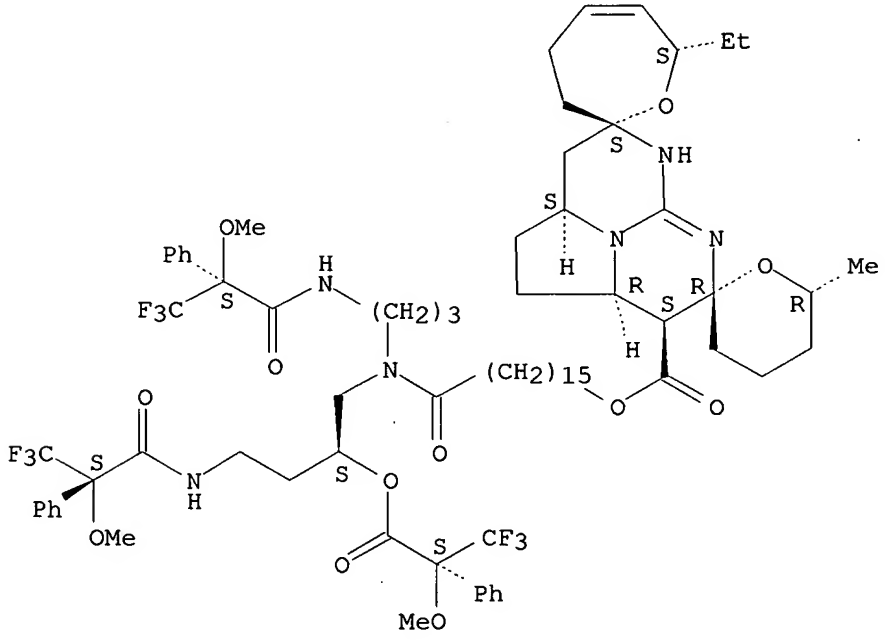
PAGE 2-A

● HCl

RN 275808-58-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2S)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, monohydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

● HCl

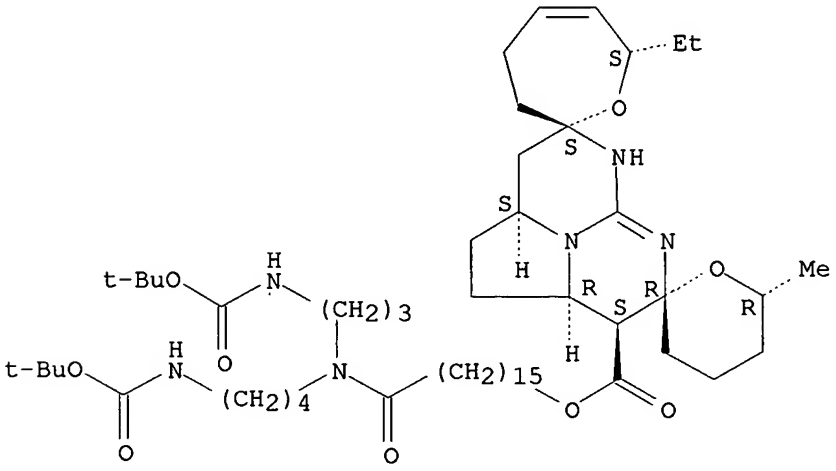
IT 162145-92-8P 162240-64-4P 275808-01-0P,
(-)-Ptilomycalin A hydrochloride 275808-29-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total synthesis of ptilomycalin A)
RN 162145-92-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 162145-91-7
CMF C55 H96 N6 O9

Absolute stereochemistry. Rotation (-).



CM 2

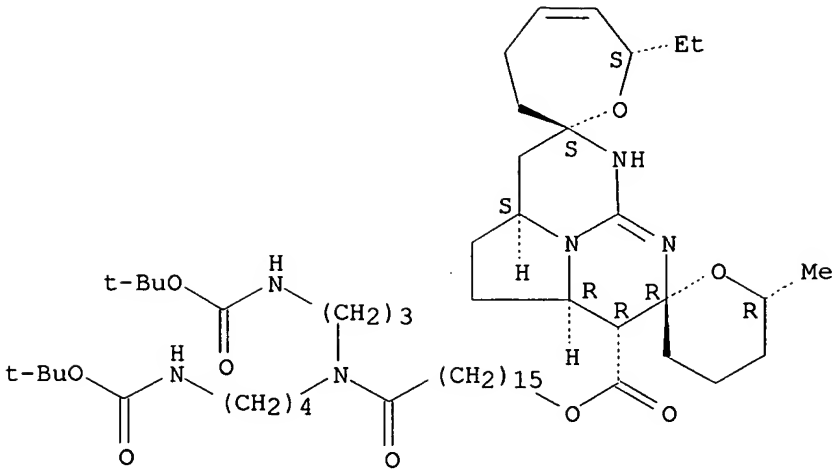
CRN 64-18-6
CMF C H2 O2

RN 162240-64-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

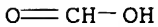
CRN 162240-63-3
CMF C55 H96 N6 O9

Absolute stereochemistry. Rotation (+).



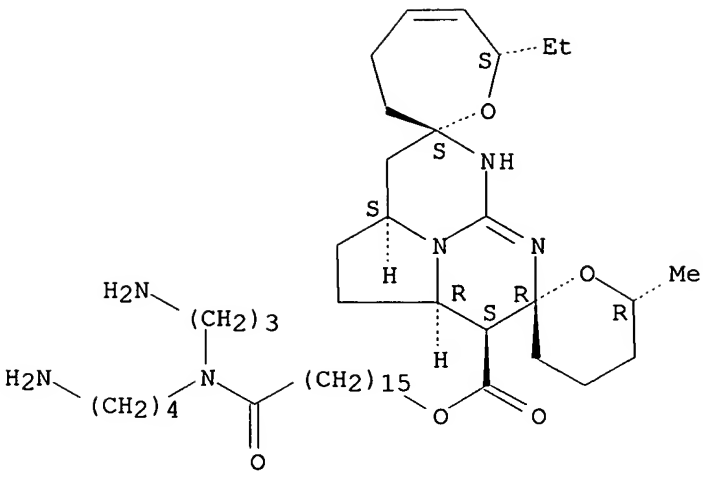
CM 2

CRN 64-18-6
CMF C H2 O2



RN 275808-01-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



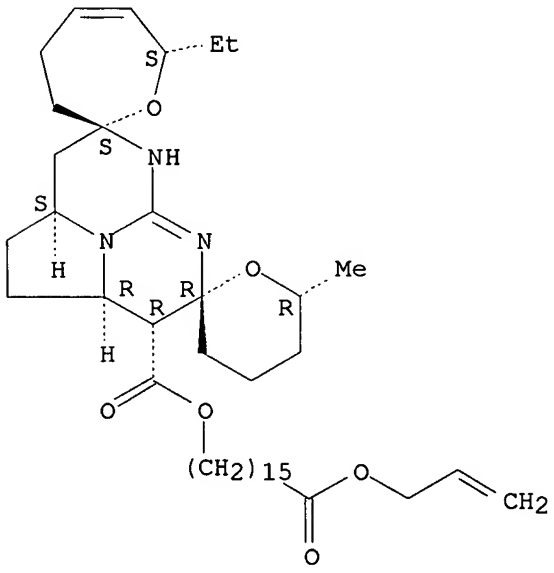
●3 HCl

RN 275808-29-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 275808-28-1
CMF C41 H67 N3 O6

Absolute stereochemistry. Rotation (+).



CM 2

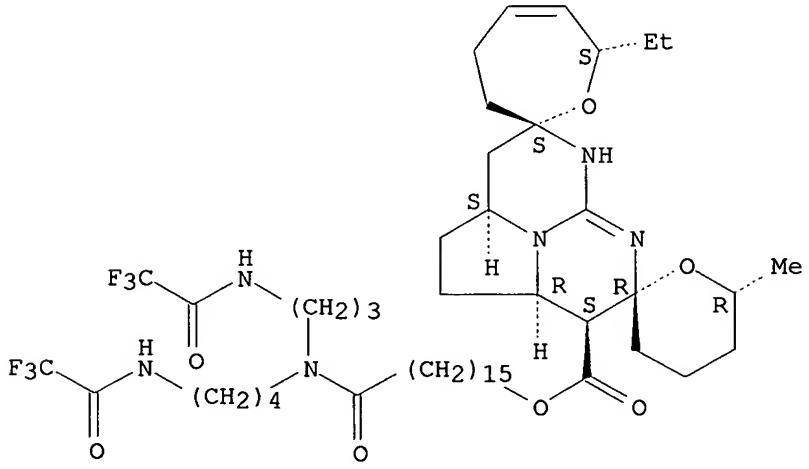
CRN 64-18-6
CMF C H2 O2

IT 125422-23-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total synthesis of ptilomycalin A)
RN 125422-23-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[4-[(trifluoroacetyl)amino]butyl][3-[(trifluoroacetyl)amino]propyl]amino]hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

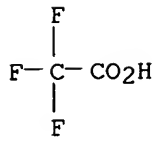
CRN 125422-22-2
CMF C49 H78 F6 N6 O7

Absolute stereochemistry. Rotation (-).



CM 2

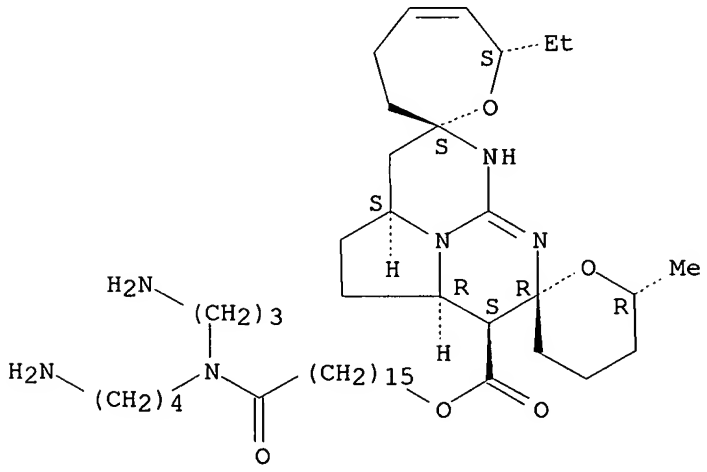
CRN 76-05-1
CMF C2 H F3 O2



RE.CNT 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

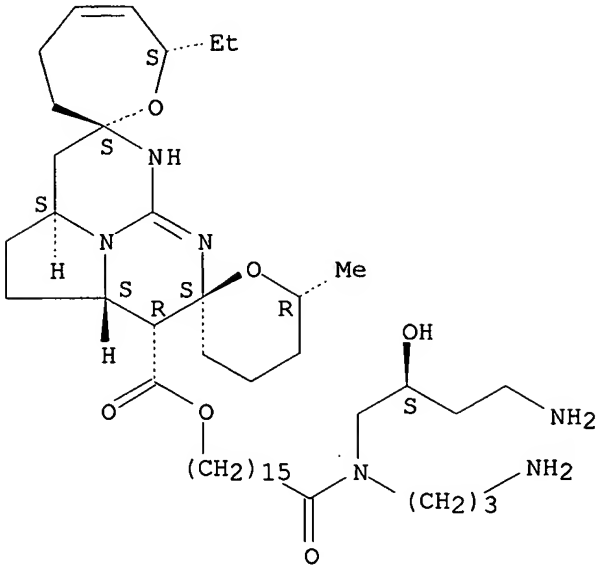
L11 ANSWER 22 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:82453 CAPLUS
DN 132:251285
TI Practical and stereoselective synthesis of a pentacyclic guanidine system: synthetic studies toward ptilomycalin A and related compounds
AU Nagasawa, Kazuo; Georgieva, Angelina; Nakata, Tadashi
CS RIKEN (The Institute of Physical and Chemical Research), Wako, 351-0198, Japan
SO Tetrahedron (1999), Volume Date 2000, 56(2), 187-192
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 132:251285
AB Sym. pentacyclic guanidine compds., e.g. I, were synthesized based on the construction of 2,5-disubstituted pyrrolidines via sequential 1,3-dipolar cycloaddn. and the formation of pentacyclic guanidine via guanylation followed by double N,O-acetalization. The present synthesis will provide a potential route for the synthesis towards ptilomycalin A and 13,14,15-isocrambescidin 800.
IT 124512-47-6P 151121-78-7P, Isocrambescidin 800
RL: PNU (Preparation, unclassified); PREP (Preparation)
(practical and stereoselective synthesis of a pentacyclic guanidine system: synthetic studies toward ptilomycalin A and related compds.)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 151121-78-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

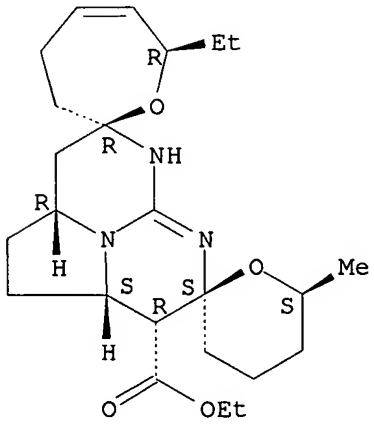
Absolute stereochemistry. Rotation (-).



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 23 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:44102 CAPLUS
DN 132:191911
TI Novel polycyclic guanidine alkaloids from two marine sponges of the genus Monanchora
AU Braekman, J. C.; Daloze, D.; Tavares, R.; Hajdu, E.; Van Soest, R. W. M.
CS Laboratory of Bio-organic Chemistry Department of Organic Chemistry Faculty of Sciences, University of Brussels, Brussels, 1050, Belg.
SO Journal of Natural Products (2000), 63(2), 193-196
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
AB Two marine sponges of the genus Monanchora (Poecilosclerida, Crambeidae) have been found to contain new polycyclic guanidine alkaloids bearing the (5,6,8b)-triazaperhydroacenaphthylene skeleton. Their structures have been determined by detailed spectroscopic anal. Dehydrobatzelladine C (I) has been isolated from M. arbuscula and crambescidins 359 (II) and 431 (III) from M. unguiculata. The chemotaxonomic implications of these findings are discussed.
IT 259734-00-4P, Crambescidin 431
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(polycyclic guanidine alkaloids from marine sponges of genus Monanchora)
RN 259734-00-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, ethyl ester, (2R,2''S,2'aR,6''S,7R,8'R,8'aS)-rel-(+)- (9CI) (CA INDEX NAME)

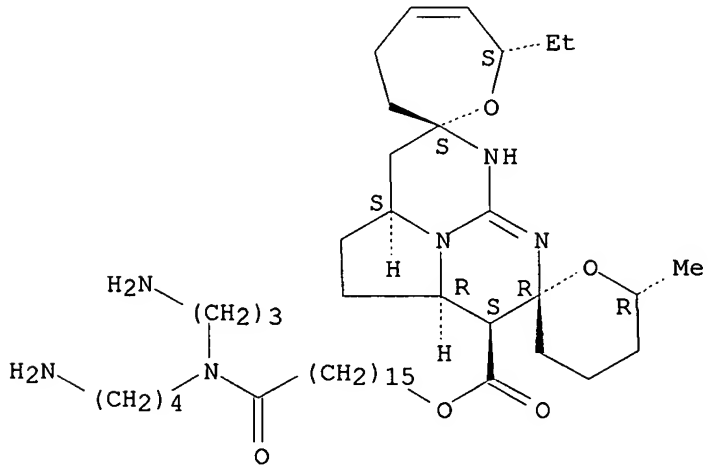
Rotation (+). Absolute stereochemistry unknown.
Currently available stereo shown.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 24 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:21284 CAPLUS
DN 132:234443
TI The guanidine metabolites of Ptilocaulis spiculifer and related compounds; isolation and synthesis
AU Heys, Laura; Moore, Christopher G.; Murphy, Patrick J.
CS Dep. Chem., University of Wales, Bangor, Gwynedd, LL57 2UW, UK
SO Chemical Society Reviews (2000), 29(1), 57-67
CODEN: CSRVBR; ISSN: 0306-0012
PB Royal Society of Chemistry
DT Journal; General Review
LA English
AB A review with 33 refs. Marine natural products possessing guanidine functionalities display a considerable array of biol. activity and not surprisingly have attracted considerable synthetic interest. This review discusses the isolation of several guanidine containing metabolites, primarily from the sponge Ptilocaulis spiculifer, but also from other marine organisms. It also explores the synthetic methodologies adopted for their preparation and speculates on the structural similarity of the metabolite ptilomycalin A to abiotic guanidine based anionic receptor mols.
IT 124512-47-6P, Ptilomycalin A
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and synthesis of guanidine metabolites of Ptilocaulis spiculifer and related compds.)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

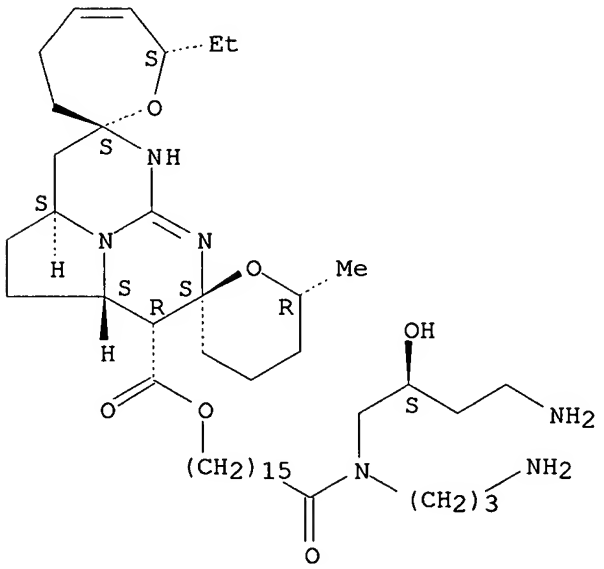
Absolute stereochemistry. Rotation (-).



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 25 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:422850 CAPLUS
DN 131:286685
TI Enantioselective Total Synthesis of 13,14,15-Isocrambescidin 800
AU Coffey, D. Scott; McDonald, Andrew I.; Overman, Larry E.; Stappenbeck, Frank
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Journal of the American Chemical Society (1999), 121(29), 6944-6945
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:286685
AB The first enantioselective total synthesis of 13,14,15-isocrambescidin 800, a rare member of the crambescidin family, was accomplished via the tethered-Biginelli condensation of the guanidino aminal intermediate of I with II and the absolute configuration of the hydroxyspermidine side chain was established as S.
IT 151121-78-7P, Isocrambescidin 800 246266-20-6P 246266-22-8P 246516-57-4P 246851-97-8P, (-)-13,14,15-Isocrambescidin 800 trihydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective preparation of 13,14,15-isocrambescidin 800)
RN 151121-78-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)-(9CI) (CA INDEX NAME)

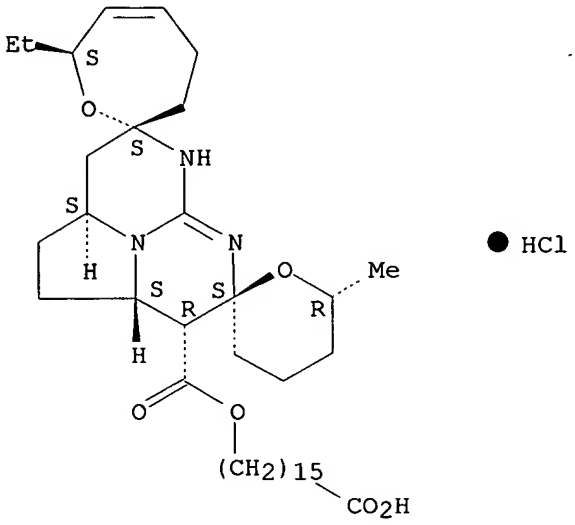
Absolute stereochemistry. Rotation (-).



RN 246266-20-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

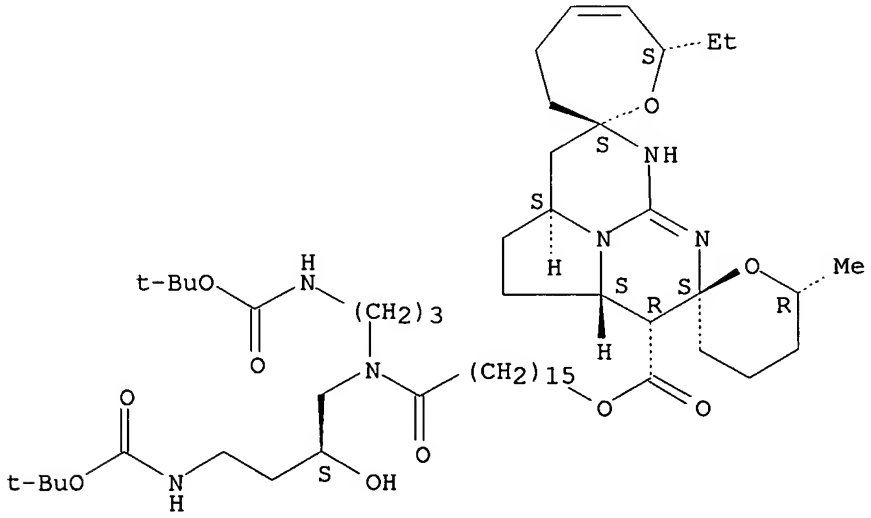


RN 246266-22-8 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxybutyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

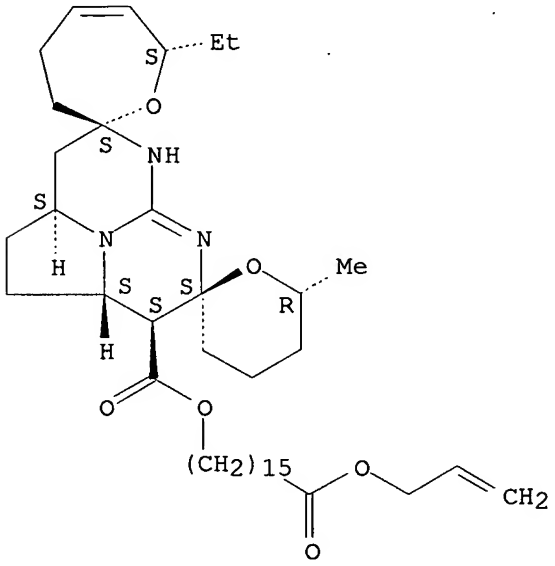


PAGE 2-A

● HCl

RN 246516-57-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

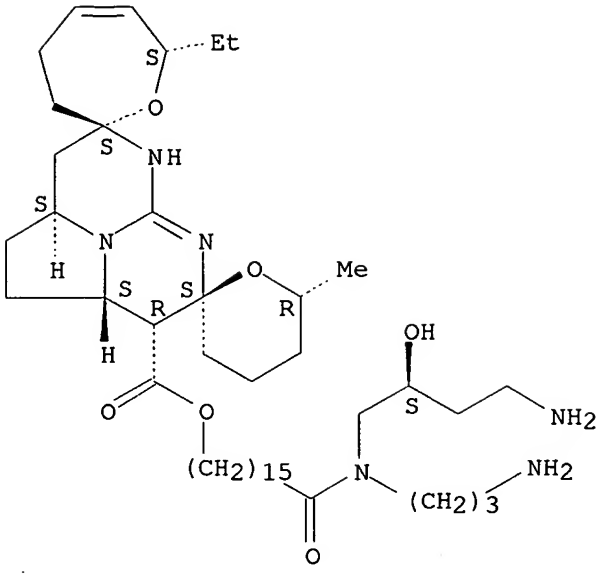
Absolute stereochemistry. Rotation (-).



● HCl

RN 246851-97-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



●3 HCl

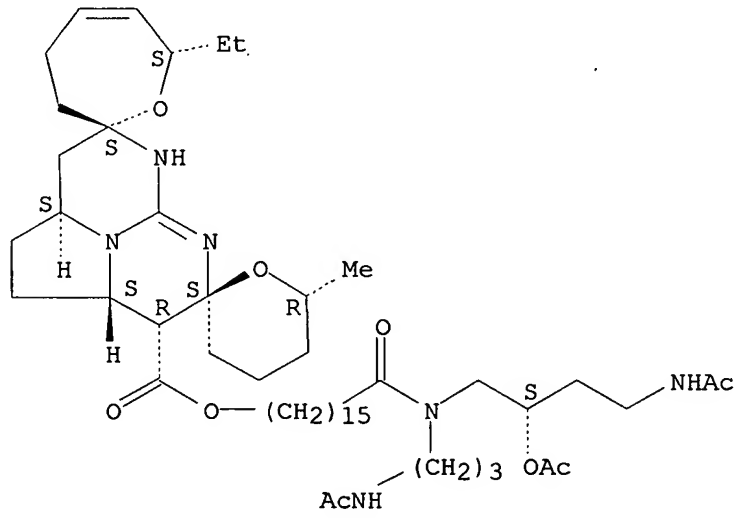
IT 246266-23-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective preparation of 13,14,15-isocrambescidin 800)

RN 246266-23-9 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, monohydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

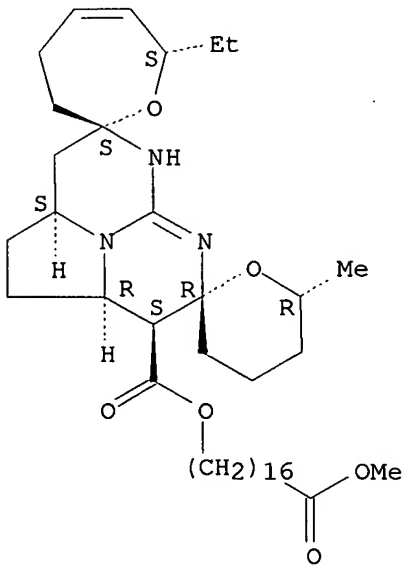


● HCl

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 26 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:287446 CAPLUS
DN 131:71418
TI Neofolitispates, pentacyclic guanidine alkaloids from the sponge Neofolitispa dianchora
AU Venkateswarlu, Y.; Reddy, M. Venkata Rami; Ramesh, P.; Rao, J. Venkateswara
CS Organic Chemistry Division-I and Toxicology Division, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1999), 38B(2), 254-256
CODEN: IJSBDB; ISSN: 0376-4699
PB National Institute of Science Communication, CSIR
DT Journal
LA English
AB Neofolitispates 1-3 (I, n = 14, 13, 12), the pentacyclic guanidine alkaloids have been isolated from the sponge Neofolitispa dianchora and characterized by spectral studies. These compds. show antiviral activity against Hepatitis-B virus.
IT 229160-50-3, Neofolitispate 1 229160-52-5, Neofolitispate 3
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(neofolitispates, pentacyclic guanidine alkaloids from sponge Neofolitispa dianchora)
RN 229160-50-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 17-methoxy-17-oxoheptadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

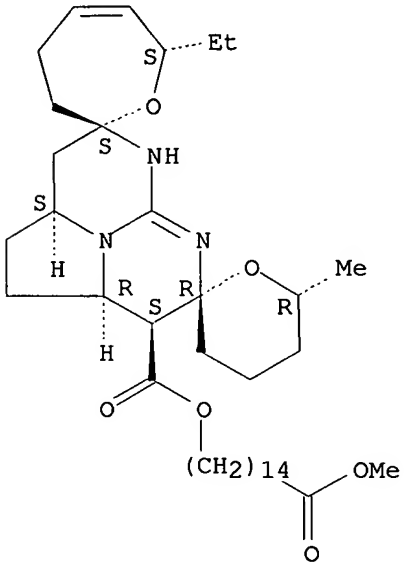
Absolute stereochemistry.



RN 229160-52-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-methoxy-15-oxopentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

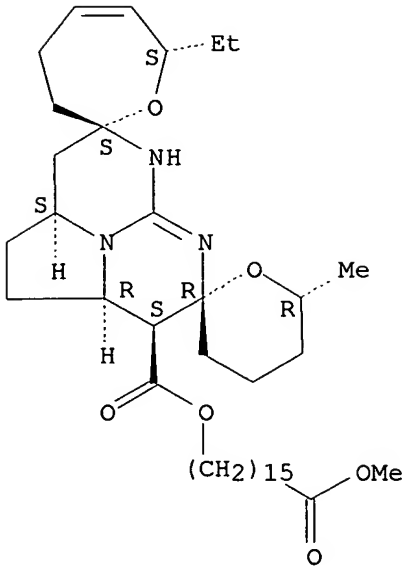


IT 229160-51-4P, Neofolitispate 2
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(neofolitispates, pentacyclic guanidine alkaloids from sponge Neofolitispa dianchora)

RN 229160-51-4 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-methoxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

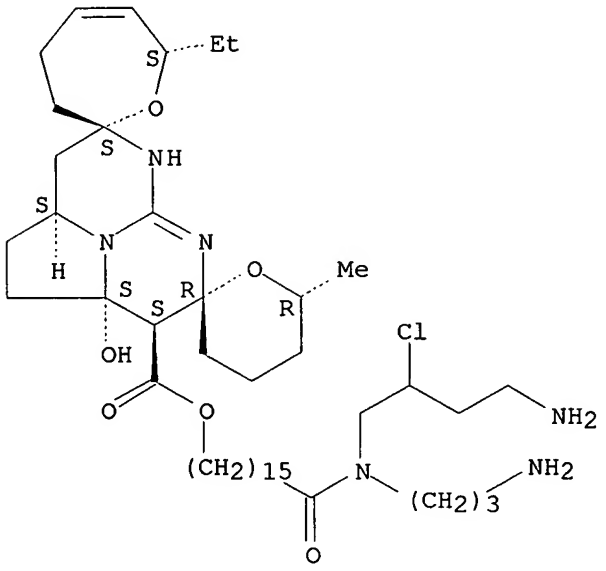
L11 ANSWER 27 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:706210 CAPLUS
DN 129:288014
TI Crambescidin isolation and structural characterization and antimicrobial and cytotoxic activity from marine sponge Crambe crambe
IN Shi, Jian-gong; Sun, Furong; Rinehart, Kenneth L.
PA Pharma Mar, S. A., Spain; Linek, Ernest, V.
SO PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9846575	A1	19981022	WO 1998-US7644	19980414
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 6028077	A	20000222	US 1998-58507	19980410
	CA 2286738	AA	19981022	CA 1998-2286738	19980414
	AU 9871241	A1	19981111	AU 1998-71241	19980414
	AU 752529	B2	20020919		
	EP 975606	A1	20000202	EP 1998-918287	19980414
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	BR 9808905	A	20000801	BR 1998-8905	19980414
	JP 2002516609	T2	20020604	JP 1998-544276	19980414
	NO 9905015	A	19991116	NO 1999-5015	19991014
	NO 313637	B1	20021104		
PRAI	US 1997-43327P	P	19970415		
	WO 1998-US7644	W	19980414		

AB Together with the known crambescidins and ptilomycalin A, two new minor crambescidins 834, 818 with a chlorinated spermidine unit and four new minor crambescidins 673, 687, 657 and 13,14,15-isocrambescidin 657 without a spermidine derivative unit have been obtained by FABMS guided isolation from exts. of the Mediterranean sponge Crambe crambe. Their structures were elucidated by interpretation of spectral data. In a parallel bioassay against L1210 murine leukemia cells, crambescidins 834, 818 and 657 were shown to be five times as cytotoxic as the knows crambescidin 816. Crambescidins with a spermidine or spermidine derivative unit also exhibited antimicrobial activity against Rhodotorula glutinis. Pharmaceutical formulations are also claimed.
IT 214215-50-6P, Crambescidin 834 214215-52-8P, Crambescidin 818 214215-54-0P, Crambescidin 673 214215-56-2P, Crambescidin 687 214215-58-4P, Crambescidin 657 214215-60-8P, 13,14,15-Isocrambescidin 657
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(crambescidin isolation and structural characterization and antimicrobial and cytotoxic activity from marine sponge Crambe crambe)
RN 214215-50-6 CAPLUS

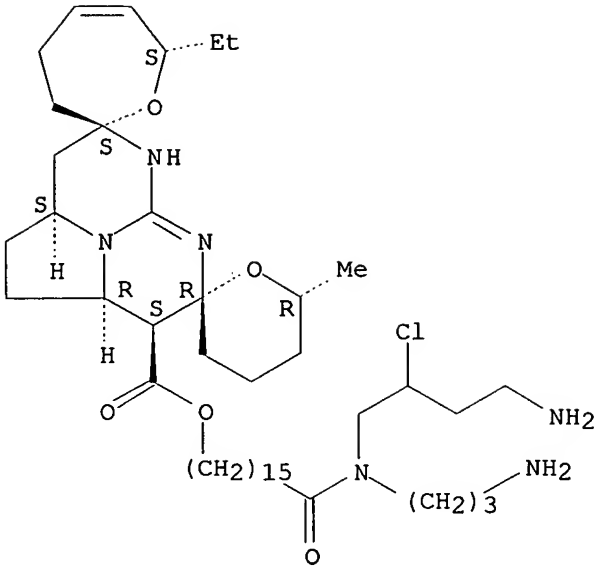
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[(4-amino-2-chlorobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Currently available stereo shown.



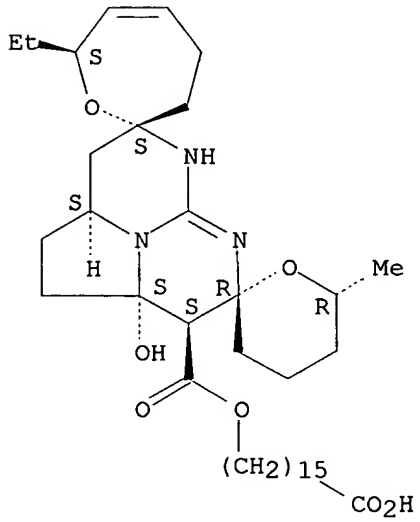
RN 214215-52-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-amino-2-chlorobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Currently available stereo shown.



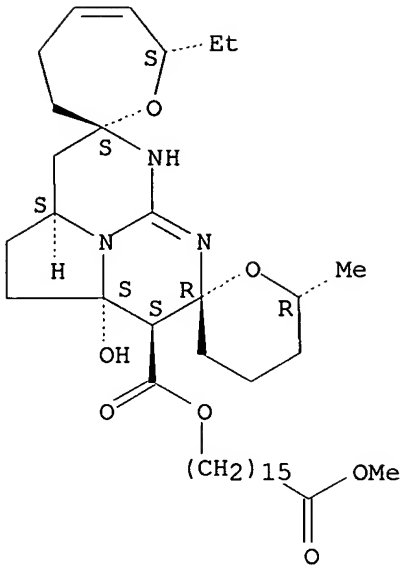
RN 214215-54-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



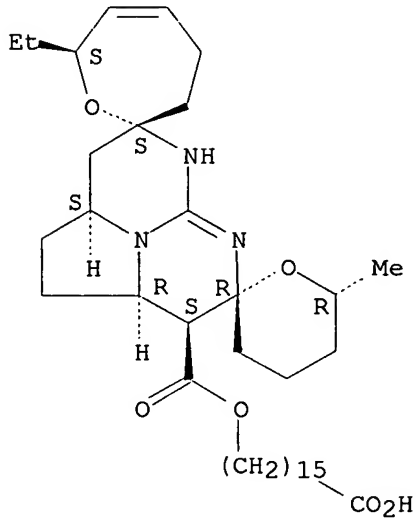
RN 214215-56-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-methoxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



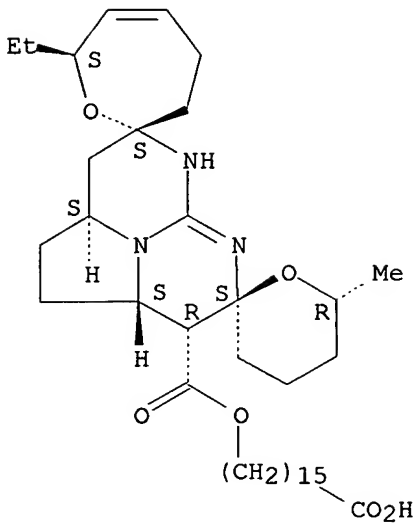
RN 214215-58-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 214215-60-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 15-carboxypentadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

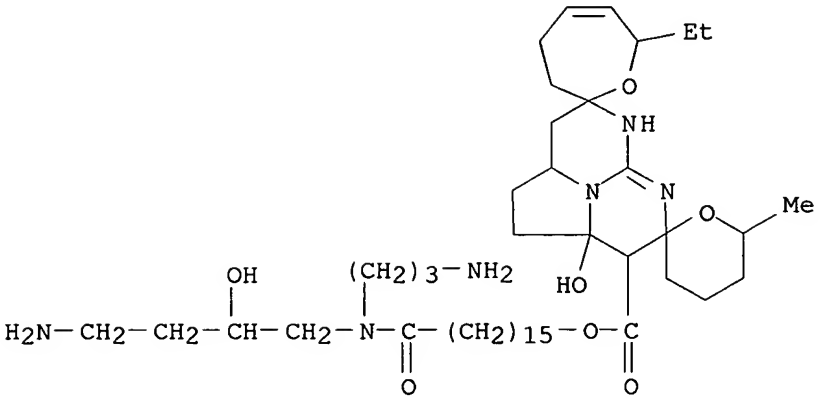
L11 ANSWER 28 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:392098 CAPLUS
DN 129:38964
TI Crambescidins: new antiviral and cytotoxic compounds from the sponge Crambe crambe
IN Rinehart, Kenneth L.; Jares-Erijman, Elizabeth A.
PA PharmaMar, S.A., Spain
SO U.S., 19 pp., Cont. of U. S. Ser. No. 944,152.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5756734	A	19980526	US 1995-476871	19950607
	US 5952332	A	19990914	US 1998-40580	19980318
PRAI	US 1992-944152	A1	19920911		
	US 1995-476871	A1	19950607		

AB The present invention is directed to several novel compds. isolated from the sponge Crambe crambe, and designated herein as Crambescidin 816 (I, R1 = R2 = OH, n = 13), Crambescidin 830 (I, R1 = R2 = OH, n = 14), Crambescidin 844 (I, R1 = R2 = OH, n = 15), and Crambescidin 800 (I, R1 = H, R2 = OH, n = 13), as well as several derivs. thereof. The 816, 830, 844 and 800 compds. are four preferred species of complex pentacyclic guanidines linked by a linear ω-hydroxy fatty acid to a hydroxyspermidine, that have been obtained by a bioassay-guided isolation procedure, involving solvent partition and chromatog. on Sephadex LH-20, cyano, and C-18 columns, from exts. of the red, encrusting sponge Crambe crambe (Order Poecilosclerida, Family Esperiopsidae).

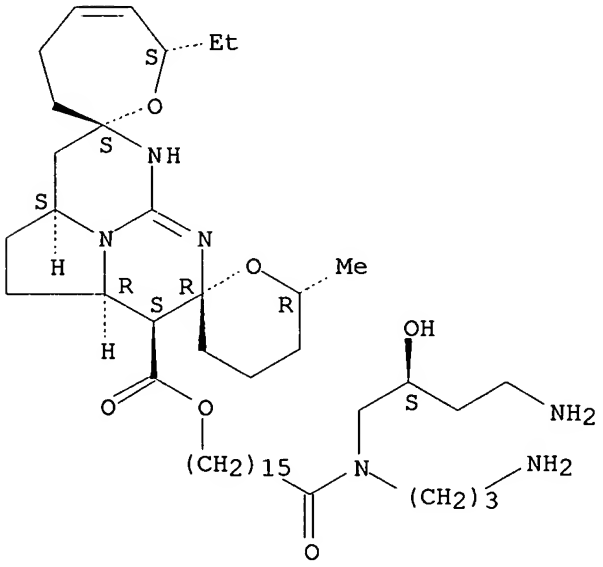
IT 135257-45-3P, Crambescidin 816 135257-46-4P, Crambescidin 800
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(crambescidins, new antiviral and cytotoxic compds. from sponge Crambe crambe)

RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



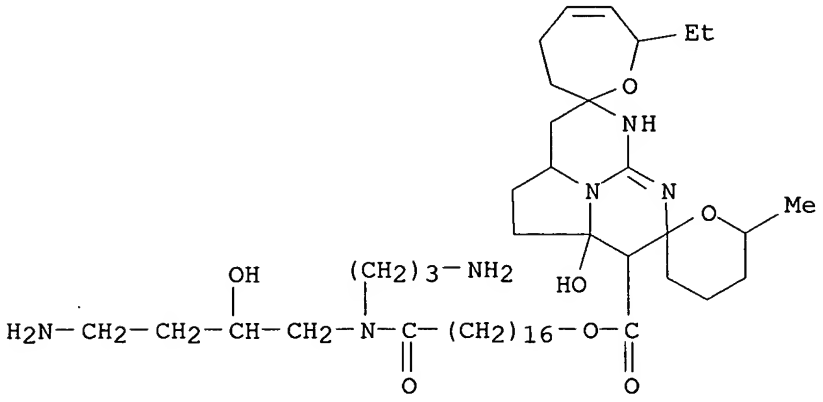
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



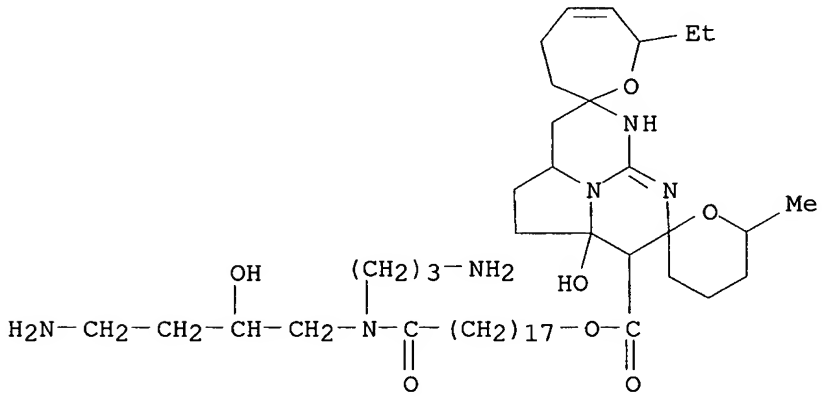
IT 135257-47-5P, Crambescidin 830 135283-73-7P, Crambescidin 844
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(crambescidins, new antiviral and cytotoxic compds. from sponge Crambe crambe)
RN 135257-47-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-

[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 17-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-17-oxoheptadecyl ester (9CI) (CA INDEX NAME)



RN 135283-73-7 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 18-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-18-oxooctadecyl ester (9CI) (CA INDEX NAME)



IT 208395-86-2P 208395-90-8P

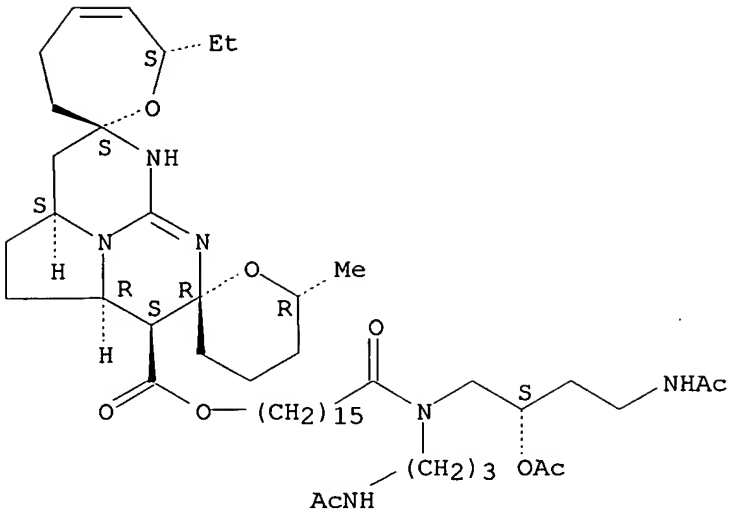
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(crambescidins, new antiviral and cytotoxic compds. from sponge Crambe crambe)

RN 208395-86-2 CAPLUS

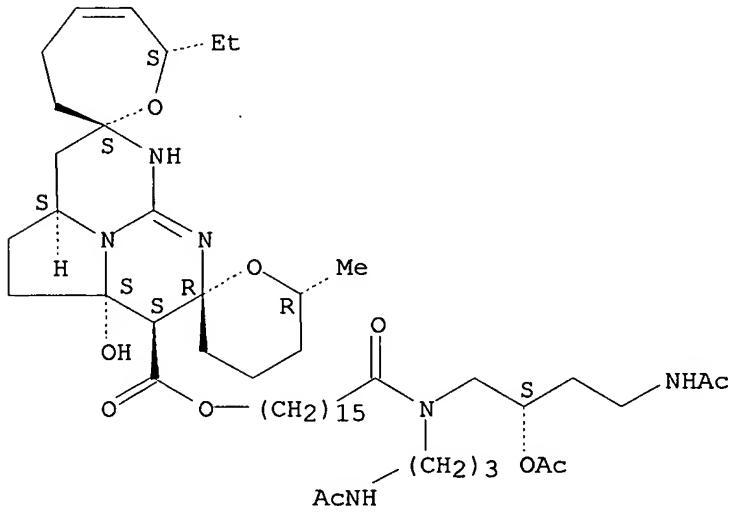
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 208395-90-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-(acetylamino)-2-(acetyloxy)butyl][3-(acetylamino)propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

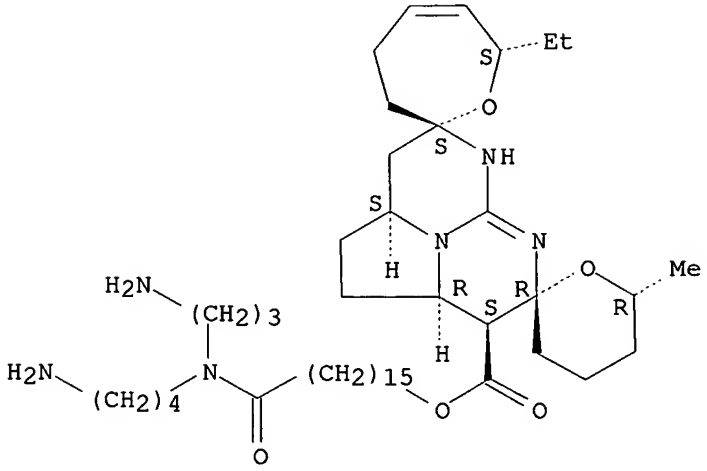
Absolute stereochemistry.



IT 124512-47-6, Ptilomycalin a
RL: PRP (Properties)
(crambescidins, new antiviral and cytotoxic compds. from sponge Crambe crambe)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-

oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

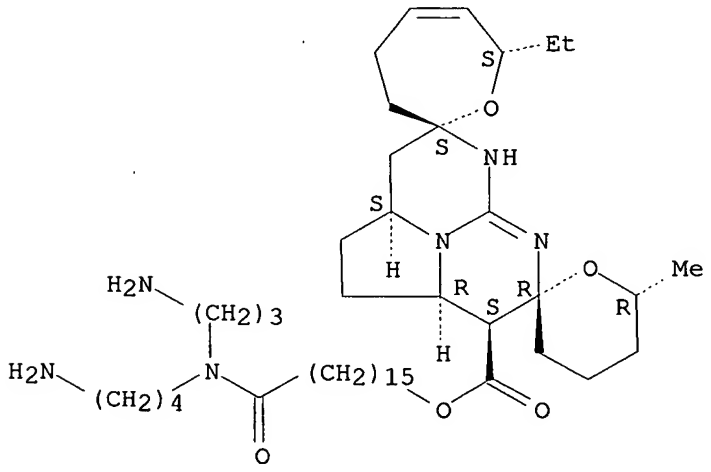
Absolute stereochemistry. Rotation (-).



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 29 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:288578 CAPLUS
DN 128:330412
TI Strategies for the design of biomimetic oxoanion ionophores for ion-selective electrodes
AU Ball, J. Christopher; Hutchins, Richard S.; Raposo, Cesar; Moran, Joaquin R.; Alajarin, Mateo; Molina, Pedro; Bachas, Leonidas G.
CS Dep. Chem., Univ. Kentucky, Lexington, KY, 40506-0055, USA
SO ACS Symposium Series (1998), 690(Polymers in Sensors), 248-256
CODEN: ACSMC8; ISSN: 0097-6156
PB American Chemical Society
DT Journal
LA English
AB Biomimetic ionophores were developed for use in ion-selective electrodes (ISEs). By mimicking the strong interactions between certain biol. mols. and oxoanions, ionophores were designed that demonstrate high selectivity for particular oxoanions. Ionophores based on the guanidinium functional group and a derivatized urea group were prepared ISEs for hydrogen sulfite, salicylate, and ibuprofen based on these ionophores are described.
IT 124512-47-6, Ptilomycalin A
RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)
(hydrogen sulfite, salicylate, and ibuprofen determination by ion-selective electrodes based on biomimetic ionophores)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

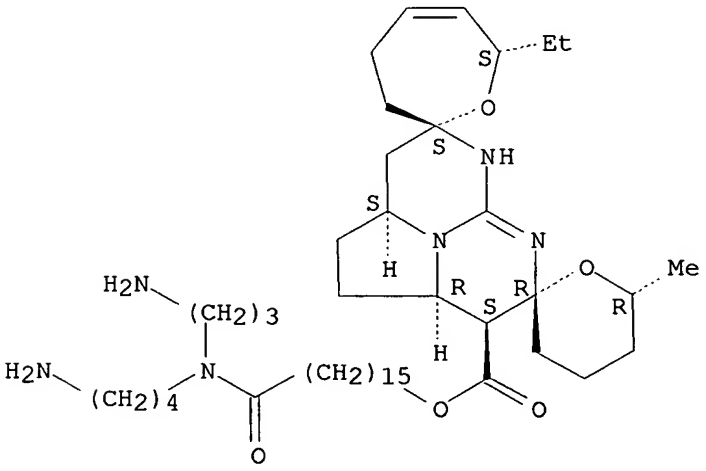
Absolute stereochemistry. Rotation (-).



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

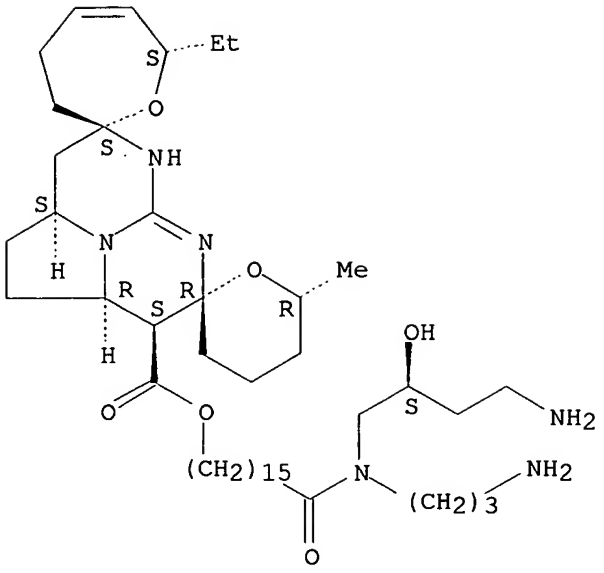
L11 ANSWER 30 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:199700 CAPLUS
DN 128:215457
TI In vitro antiviral activity on dengue virus of marine natural products
AU Laille, M.; Gerald, F.; Debitus, C.
CS Institut Pasteur, Noumea, 98845, New Caledonia
SO Cellular and Molecular Life Sciences (1998), 54(2), 167-170
CODEN: CMLSFI; ISSN: 1420-682X
PB Birkhaeuser Verlag
DT Journal
LA English
AB Metabolites isolated from marine invertebrates, callipeltin A, crambescidin, tilomycalin A, celeromycalin, gymnochrome B, gymnochrome D, and isogymnochrome D were tested on a in vitro bioassay using the dengue virus 1. Only gymnochrome D and isogymnochrome D isolated from the living fossil crinoid Gymnocrinus richeri are highly potent dengue antiviral agents.
IT 124512-47-6, Ptilomycalin A 135257-46-4, Crambescidin 800 163597-72-6, Celeromycalin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(in vitro antiviral activity on dengue virus of marine natural products)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



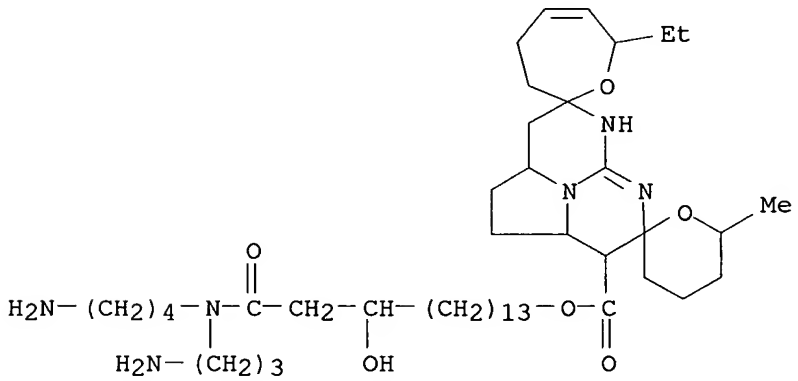
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



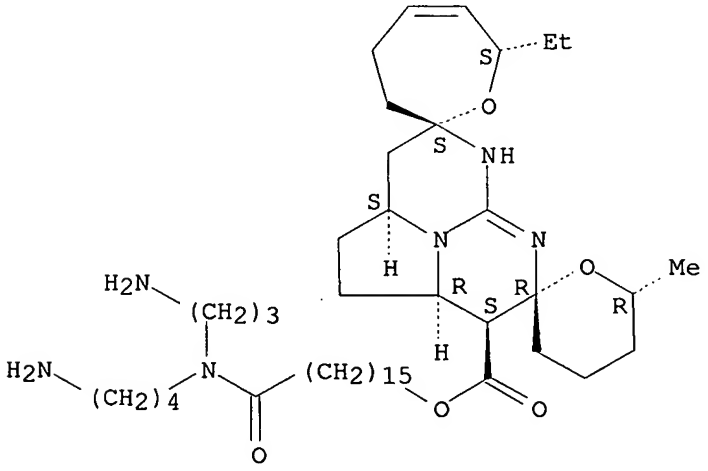
RN 163597-72-6 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (14R)-16-[(4-aminobutyl)(3-aminopropyl)amino]-14-hydroxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)



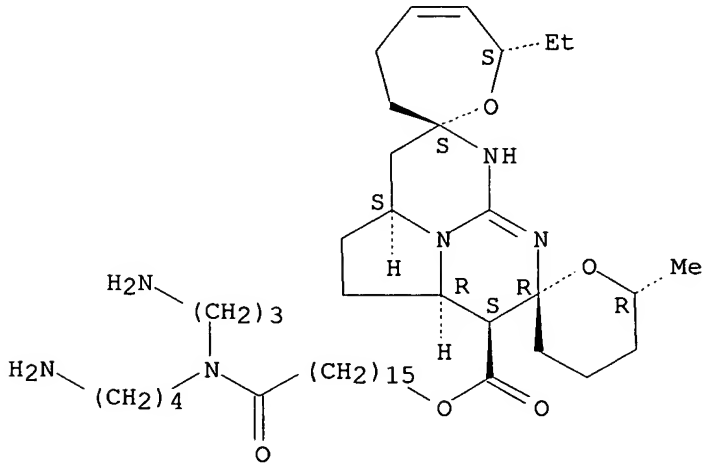
L11 ANSWER 31 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:526062 CAPLUS
DN 125:215428
TI Ptilomycalin A, a novel Na+,K+- or Ca2+-ATPase inhibitor, competitively interacts with ATP at its binding site
AU Ohizumi, Yasushi; Sasaki, Susumu; Kusumi, Takenori; Ohtani, Ikuko I.
CS Department of Pharmaceutical Molecular Biology, Faculty of Pharmaceutical Sciences, Tohoku University, Aoba, Aramaki, Aoba-ku, Sendai, Japan
SO European Journal of Pharmacology (1996), 310(1), 95-98
CODEN: EJPHAZ; ISSN: 0014-2999
PB Elsevier
DT Journal
LA English
AB Ptilomycalin A inhibited the brain Na+,K+-ATPase and Ca2+ -ATPase from skeletal sarcoplasmic reticulum with an IC50 value of 2 μM and 10 μM, resp. Kinetic anal. of the inhibitory effects of ptilomycalin A suggests that the inhibition of Na+,K+-ATPase is a competitive-, an uncompetitive- and an anticompetitive-type with respect to ATP, Na+ and K+, resp. The inhibition of Ca2+-ATPase by ptilomycalin A is a competitive- or an uncompetitive-type with respect to ATP or Ca2+, resp. These results suggest that ptilomycalin A interacts with ATP at the ATP binding site of Na+,K+-ATPase or Ca2+-ATPase. Ptilomycalin A has become a useful biochem. tool for clarifying the ATP binding site in both enzymes.
IT 124512-47-6, Ptilomycalin A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(ptilomycalin A competitively interacts with ATP-binding sites of Na+,K+- and Ca2+-ATPase)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



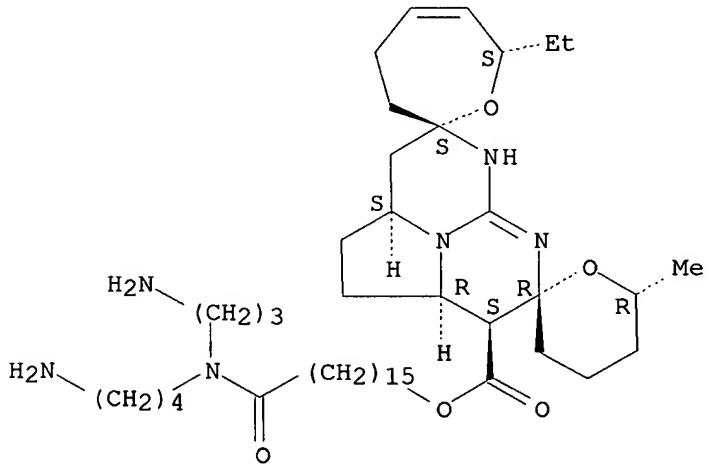
L11 ANSWER 32 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:376459 CAPLUS
DN 125:114928
TI Biomimetic model studies towards ptilomycalin A
AU Murphy, Patrick J.; Williams, Harri Lloyd; Hibbs, David E.; Hursthouse, Michael B.; Malik, K. M. Abdul
CS Dep. Chem., Univ. Wales, Gwynedd, LL57 2UW, UK
SO Tetrahedron (1996), 52(24), 8315-8332
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
OS CASREACT 125:114928
AB Model compds., such as tetracycles I and pentacycles II (m = n = 0; m = n = 1; m = 0, n = 1), were prepared to illustrate a biomimetic approach to the synthesis of the guanidine containing natural product ptilomycalin A.
IT 124512-47-6P, Ptilomycalin A
RL: PNU (Preparation, unclassified); PREP (Preparation)
(biomimetic model studies towards the synthesis ptilomycalin A)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



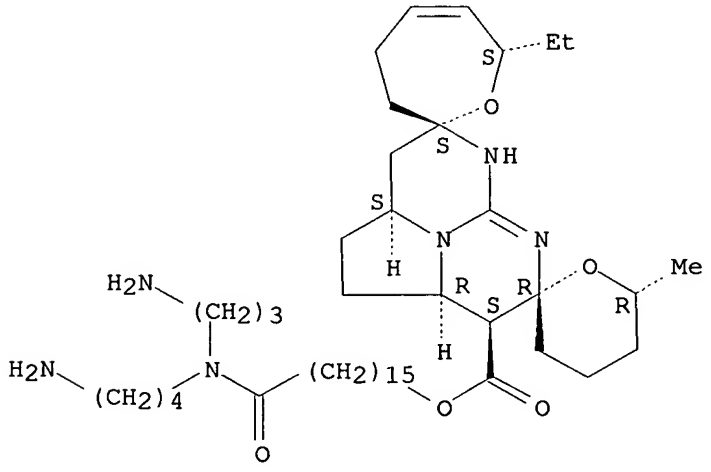
L11 ANSWER 33 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:270070 CAPLUS
DN 125:11195
TI An antibody catalyzed ester hydrolysis and a synthetic approach towards agelastatin A
AU Anderson, Glen Thomas
CS Pennsylvania State Univ., University Park, PA, USA
SO (1996) 118 pp. Avail.: Univ. Microfilms Int., Order No. DA9612684
From: Diss. Abstr. Int., B 1996, 56(12), 6741
DT Dissertation
LA English
AB Unavailable
IT 124512-47-6P, Ptilomycalin a
RL: PNU (Preparation, unclassified); PREP (Preparation)
(antibody catalyzed ester hydrolysis and a synthetic approach towards agelastatin a)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



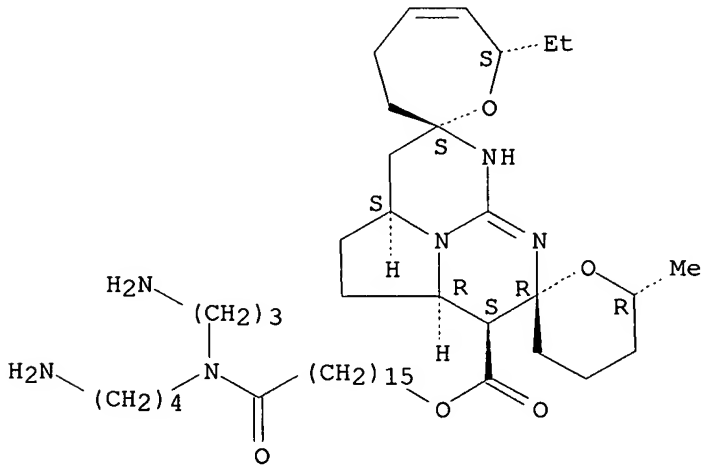
L11 ANSWER 34 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:154421 CAPLUS
DN 124:317586
TI Crystallographic evidence for the proposed host behavior of ptilomycalin A
AU Murphy, Patrick J.; Williams, Harri Lloyd; Hibbs, David E.; Hursthouse, Michael B.; Malik, K. M. Abdul
CS Dep. Chem., Univ. Wales, Bangor, LL57 2UW, UK
SO Chemical Communications (Cambridge) (1996), (3), 445-7
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB The X-ray crystal structures of model compds, e.g. pentacyclic guanidine I, were determined and used as evidence to support proposed anionic recognition in the alkaloid ptilomycalin A.
IT 124512-47-6, Ptilomycalin A
RL: PRP (Properties)
(crystallog. evidence for the proposed host behavior of ptilomycalin A)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



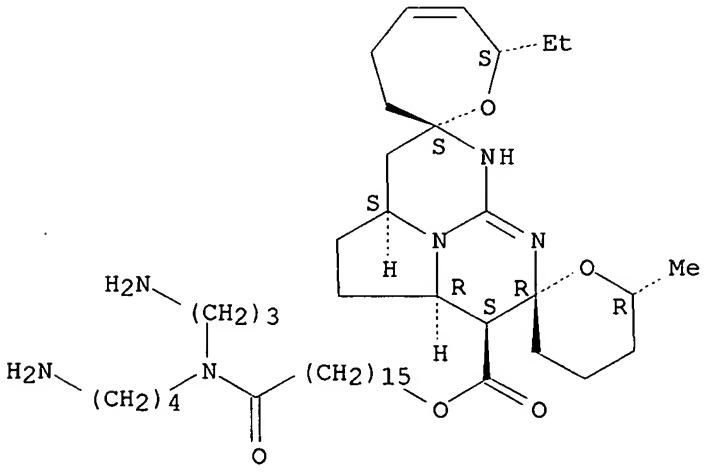
L11 ANSWER 35 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:102088 CAPLUS
DN 124:232861
TI Synthesis of bicyclic guanidines from pyrrolidin-2-one
AU Louwrier, Saskia; Tuynman, Antonin; Hiemstra, Henk
CS Amsterdam Inst. Mol. Studies, Univ. Amsterdam, Amsterdam, 1018 WS, Neth.
SO Tetrahedron (1996), 52(7), 2629-46
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
OS CASREACT 124:232861
AB The syntheses of three bicyclic guanidines I (R = Ph, R1 = H; R = n-Pr, R1 = H; R = Me, R1 = CO2Me), as model compds. for the guanidine alkaloid ptilomycalin A, are described. The guanidines are prepared from pyrrolidin-2-one via an N-acyliminium ion coupling reaction with silyl enol ethers and a direct guanylation with bis-Boc-thiourea and HgCl2 as the key steps.
IT 124512-47-6P, Ptilomycalin A
RL: PNU (Preparation, unclassified); PREP (Preparation)
(synthesis of bicyclic guanidines as model compds. for ptilomycalin A from pyrrolidinone)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



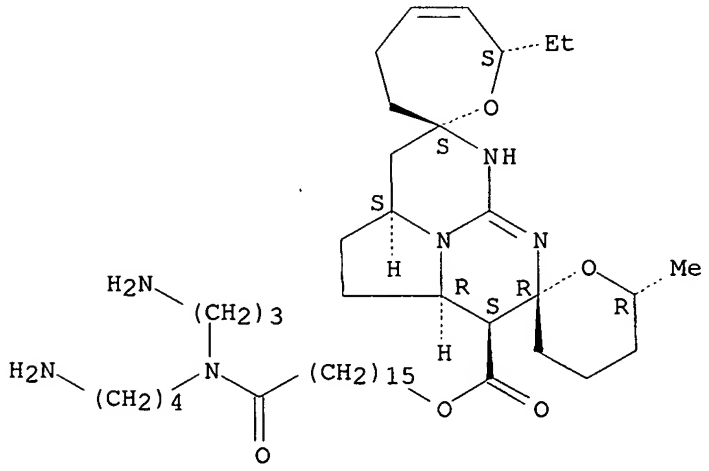
L11 ANSWER 36 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:102087 CAPLUS
DN 124:261438
TI Studies towards the synthesis of (+)-ptilomycalin A; stereoselective N-acyliminium ion coupling reactions to enantiopure C-2 substituted lactams
AU Louwrier, Saskia; Ostendorf, Martin; Boom, Arnoud; Hiemstra, Henk; Speckamp, W. Nico
CS Amsterdam Inst. Mol. Studies, Univ. Amsterdam, Amsterdam, 1018 WS, Neth.
SO Tetrahedron (1996), 52(7), 2603-28
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
OS CASREACT 124:261438
AB Highly stereoselective N-acyliminium ion coupling reactions of β-ketoester derived silyl enol ethers with enantiopure lactams derived from (S)-malic acid are reported. This reaction type is applied in the synthesis of the enantiopure C-2 substituted lactam I, a plausible intermediate in a projected synthesis of ptilomycalin A.
IT 124512-47-6P, (-)-Ptilomycalin A
RL: PNU (Preparation, unclassified); PREP (Preparation)
(stereoselective N-acyliminium ion coupling reactions to enantiopure C-2 substituted lactams directed toward synthesis of ptilomycalin A)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



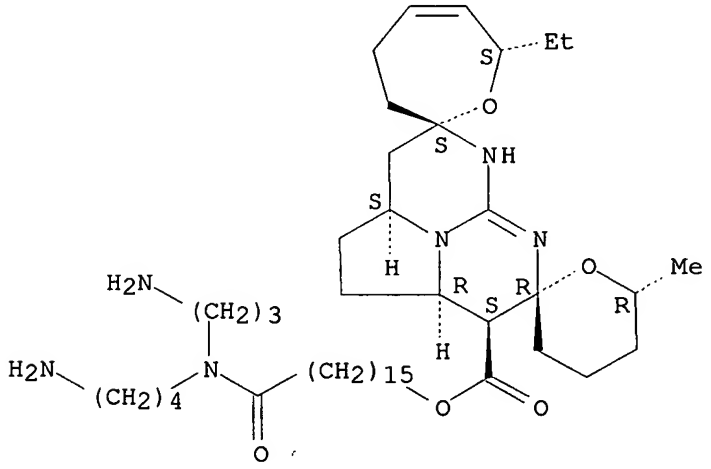
L11 ANSWER 37 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:97102 CAPLUS
DN 124:232860
TI Studies towards the synthesis of guanidine alkaloids; synthesis of a tricyclic guanidine from succinimide
AU Louwrier, Saskia; Ostendorf, Martin; Tuynman, Antonin; Hiemstra, Henk
CS Amsterdam Inst. Mol. Studies, Univ. Amsterdam, Amsterdam, 1018 WS, Neth.
SO Tetrahedron Letters (1996), 37(6), 905-8
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
OS CASREACT 124:232860
AB The synthesis of a tricyclic guanidine I as a model compound for ptilomycalin A and related guanidine alkaloids is described. The synthesis starts from succinimide and features an N-acyliminium ion coupling, an Eschenmoser sulfide-contraction and an N-guanylation as the key steps.
IT 124512-47-6P, Ptilomycalin A
RL: PNU (Preparation, unclassified); PREP (Preparation)
(synthesis of a tricyclic guanidine alkaloid model from succinimide)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



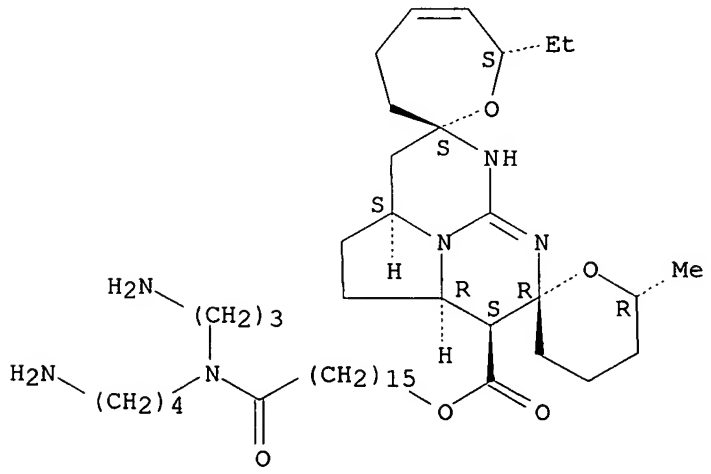
L11 ANSWER 38 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:61001 CAPLUS
DN 124:261426
TI Ptilomycalin A and other guanidinium-anion receptors
AU Koert, Ulrich
CS Univ. Marburg, Marburg, Germany
SO Nachrichten aus Chemie, Technik und Laboratorium (1995), 43(12), 1302-4, 1306-9
CODEN: NCTLDI; ISSN: 0341-5163
PB VCH
DT Journal; General Review
LA German
AB A review with 15 refs. on syntheses of the title compds.
IT 124512-47-6P, Ptilomycalin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of ptilomycalin A and other guanidinium anion-receptors)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



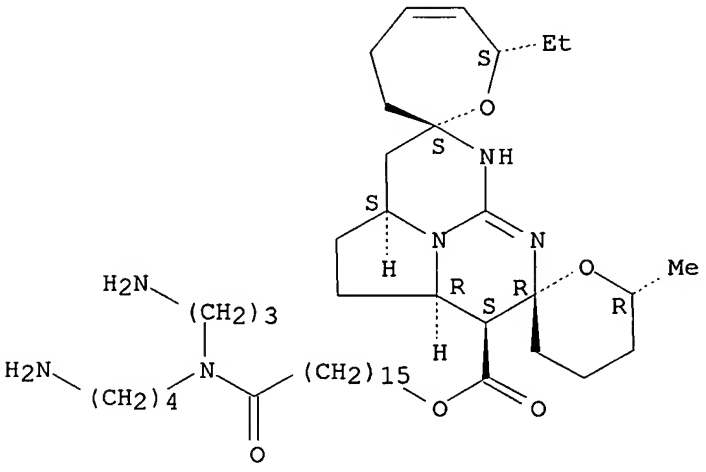
L11 ANSWER 39 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:1000242 CAPLUS
DN 124:117675
TI Catalytic Antibodies in Synthesis: Design and Synthesis of a Hapten for Application to the Preparation of a Scalemic Pyrrolidine Ring Synthon for Ptilomycalin A
AU Anderson, Glen T.; Alexander, Michael D.; Taylor, Scott D.; Smithrud, David B.; Benkovic, Stephen J.; Weinreb, Steven M.
CS Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA
SO Journal of Organic Chemistry (1996), 61(1), 125-32
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 124:117675
AB A catalytic antibody-based approach toward the synthesis of an optically active pyrrolidine ring synthon potentially useful for ptilomycalin A is described. Enantiomerically pure hapten I was designed and constructed with the eventual goal of generating antibodies for the enantioselective partial hydrolysis of a meso diester such as into a monoacid. This transition state analog possesses a phosphonate group containing the requisite oxyanionic character of the tetrahedral intermediate for ester hydrolysis. A newly developed carbamate-based linker, which was found to be much more hydrolytically stable than the commonly used glutarate ester, was developed for coupling of the hapten to a carrier protein.
IT 124512-47-6P, Ptilomycalin A
RL: PNU (Preparation, unclassified); PREP (Preparation)
(catalytic antibodies approach to synthesis of a hapten for application to preparation of a scalemic pyrrolidine ring synthon for ptilomycalin a)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



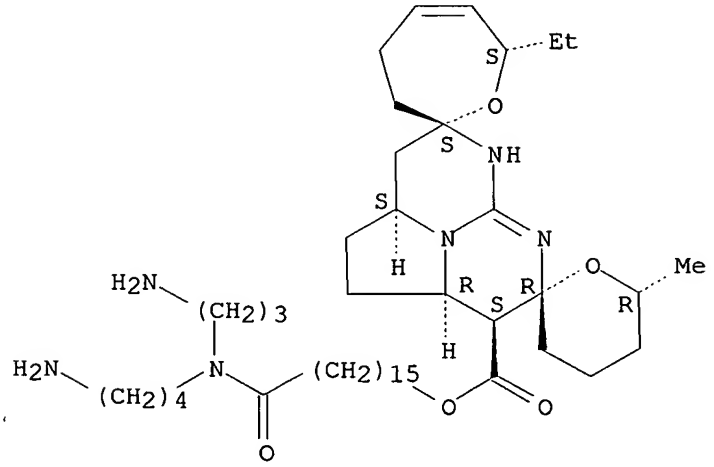
L11 ANSWER 40 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:881121 CAPLUS
DN 123:340515
TI Synthesis of a structural analog of ptilomycalin A
AU Grillot, Anne-Laure; Hart, David J.
CS Dep. Chem., Ohio State Univ., Columbus, OH, 43210, USA
SO Tetrahedron (1995), 51(42), 11377-92
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
OS CASREACT 123:340515
AB Ptilomycalin A analog I was prepared in 13 steps from BrCH2C(:CH2)CO2CMe3 via coupling of the corresponding amido alc. with the guanidiniumcarboxylate.
IT 124512-47-6DP, Ptilomycalin A, analogs
RL: PNU (Preparation, unclassified); PREP (Preparation)
(synthesis of a structural analog of ptilomycalin A)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

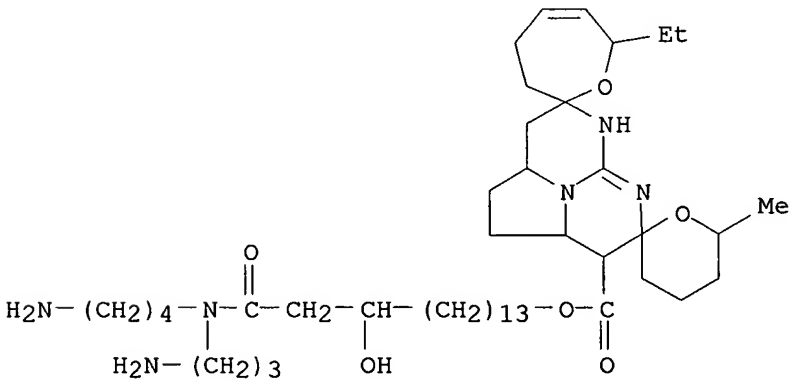


L11 ANSWER 41 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:852174 CAPLUS
DN 123:286366
TI Enantioselective total synthesis of (+)-isolaurepinnacin and enantioselective total synthesis of (-)-ptilomycalin a
AU Renhowe, Paul Allan
CS Univ. of California, Irvine, CA, USA
SO (1995) 148 pp. Avail.: Univ. Microfilms Int., Order No. DA9525158 From: Diss. Abstr. Int., B 1995, 56(3), 1429
DT Dissertation
LA English
AB Unavailable
IT 124512-47-6P, Ptilomycalin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total synthesis of (+)-isolaurepinnacin and (-)-ptilomycalin A)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

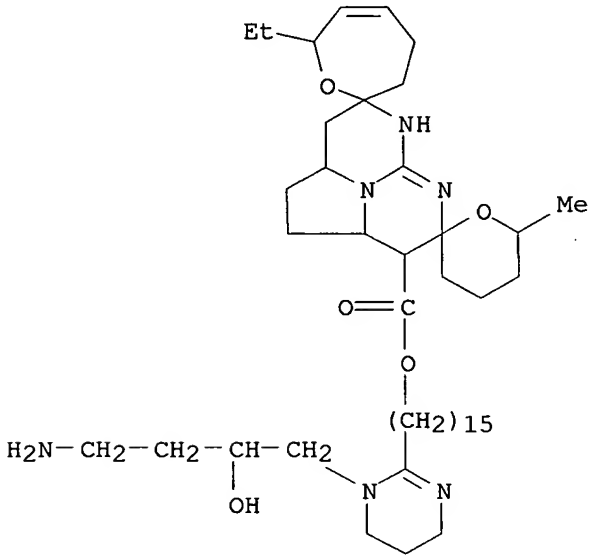


L11 ANSWER 42 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:484163 CAPLUS
DN 123:5862
TI Ptilomycalin A, crambescidin 800 and related new highly cytotoxic guanidine alkaloids from the starfishes Fromia monilis and Celerina heffernani
AU Palagiano, Elio; De Marino, Simona; Minale, Luigi; Riccio, Raffaele; Zollo, Franco; Iorizzi, Maria; Carre, Jean Baptiste; Debitus, Cecile; Lucarain, Laetitia; et al.
CS Dip. Chimica Sostanze Naturali "Federico II", Univ. Napoli, Napoli, 80131, Italy
SO Tetrahedron (1995), 51(12), 3675-82
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
AB Two novel pentacyclic guanidine alkaloids, celeromycalin and fromiamycalin, were isolated from the New Caledonian starfishes C. heffernani and F. monilis, resp. Also found in C. heffernani are the known ptilomycalin A and crambescidin 800, which latter has been also isolated from F. monilis. The new compds. exhibited an high cytotoxic activity like the previous crambescidins. These complex pentacyclic guanidines are typical sponges metabolites and their occurrence in starfishes is noteworthy. F. monilis also contained the less active component, made up from an hydroxyspermidine residue linked to a long chain ω-hydroxyacid.
IT 163597-72-6, Celeromycalin 163597-73-7, Fromiamycalin
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(celeromycalin and fromiamycalin isolation and structural characterization and activity from starfish)
RN 163597-72-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (14R)-16-[(4-aminobutyl)(3-aminopropyl)amino]-14-hydroxy-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)



RN 163597-73-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8'

,8'a-dodecahydro-6''-methyl-, 15-[1-(4-amino-2-hydroxybutyl)-1,4,5,6-tetrahydro-2-pyrimidinyl]pentadecyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β(R*),8'aα]]- (9CI) (CA INDEX NAME)

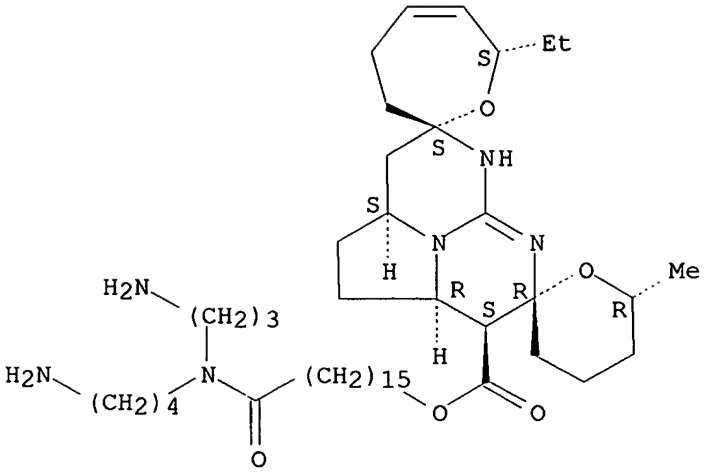


IT 124512-47-6, Ptilomycalin A 135257-46-4, Crambescidin 800
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(celeromycalin and fromiamycalin isolation and structural characterization and activity from starfish)

RN 124512-47-6 CAPLUS

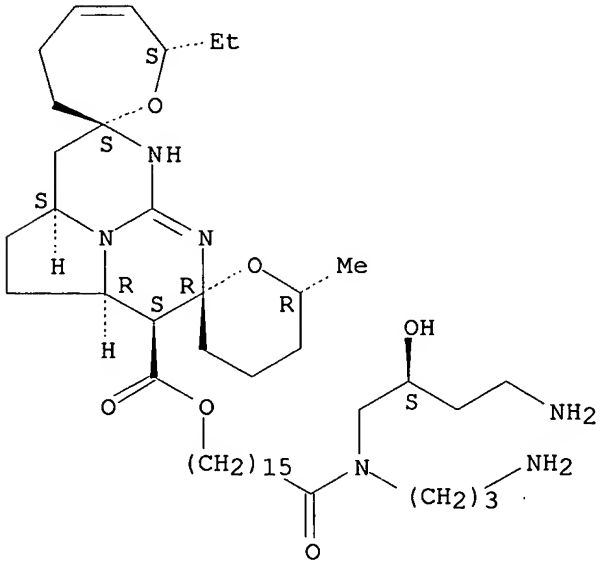
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



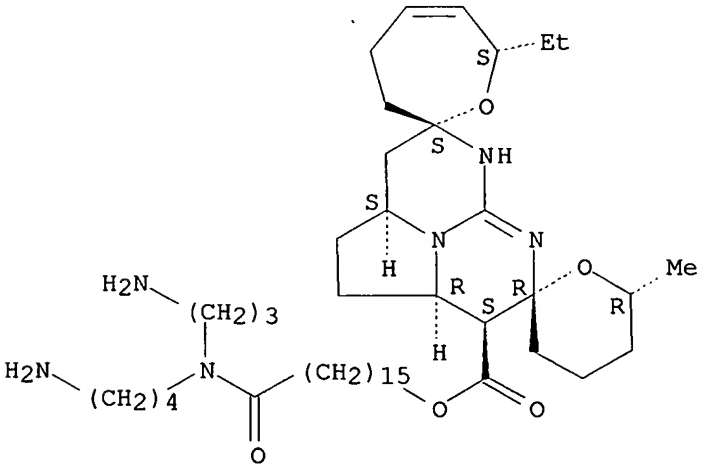
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



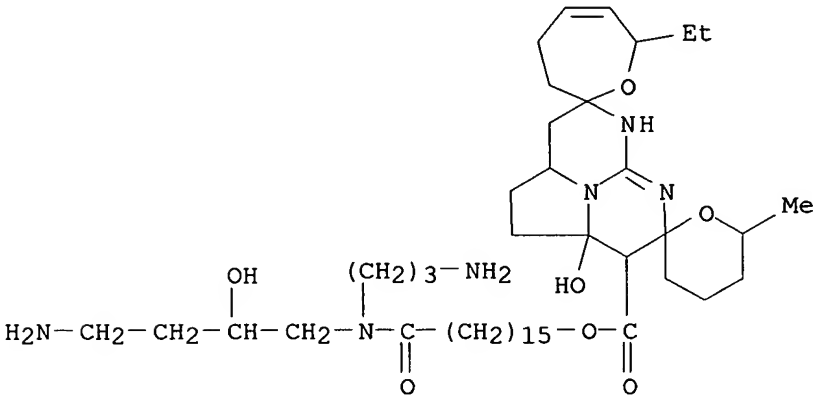
L11 ANSWER 43 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:397824 CAPLUS
DN 122:210092
TI Novel Alkaloids from the Sponge Batzella sp.: Inhibitors of HIV gp120-Human CD4 Binding
AU Patil, Ashok D.; Kumar, N. Vasant; Kokke, Wilhelmus C.; Bean, Mark F.; Freyer, Alan J.; Brosse, Charles De; Mai, Shing; Truneh, Alemseged; Carte, Brad; et al.
CS Department of Biomolecular Discovery, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406-0939, USA
SO Journal of Organic Chemistry (1995), 60(5), 1182-8
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB The Caribbean sponge Batzella sp. contains a number of guanidine alkaloids, two of which, batzelladines A (1) and B (2), inhibit the binding of HIVgp-120 to CD4 and are therefore potential inhibitors of HIV. In addition to the known metabolites ptilomycalin A (6), ptilocaulin (7), crambescin A (8), crambescidin 800 (9), and crambescidin 816 (10), Batzella sp. contains five new alkaloids, batzelladines A-E (1-5), the structures of which were elucidated by interpretation of spectral data and chemical degradation
IT 124512-47-6, Ptilomycalin A 135257-45-3, Crambescidin 816 135257-46-4, Crambescidin 800
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(novel alkaloids from sponge Batzella as inhibitors of HIV gp120)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8'

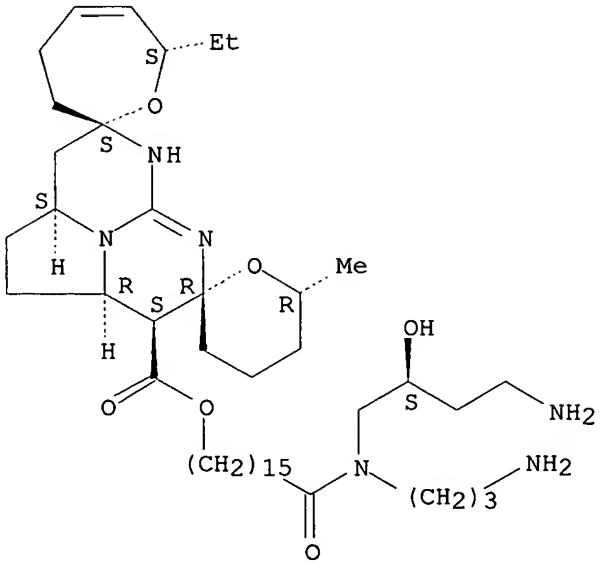
,8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



RN 135257-46-4 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

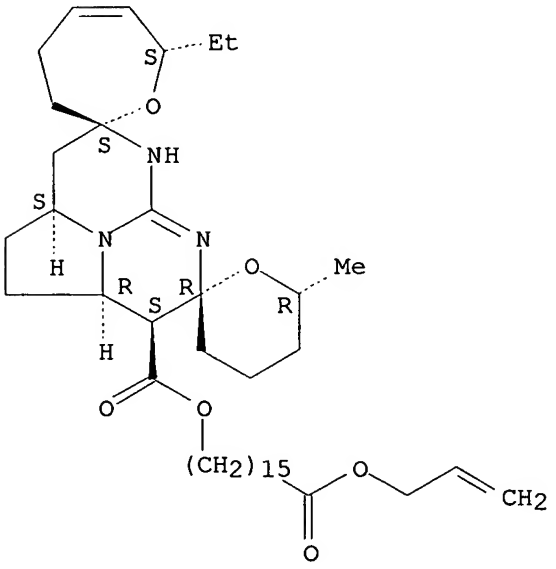


L11 ANSWER 44 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:397708 CAPLUS
DN 122:291250
TI Enantioselective Total Synthesis of (-)-Ptilomycalin A
AU Overman, Larry E.; Rabinowitz, Michael H.; Renhowe, Paul A.
CS Department of Chemistry, University of California, Irvine, CA, 92717-2025, USA
SO Journal of the American Chemical Society (1995), 117(9), 2657-8
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 122:291250
AB The total synthesis of the title compound (I) was accomplished in a convergent from three readily available enantioenriched secondary alcs.
IT 162145-90-6P 162145-92-8P 162240-64-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total synthesis of ptilomycalin A)
RN 162145-90-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-(2-propenyloxy)hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 162145-89-3
CMF C41 H67 N3 O6

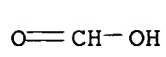
Absolute stereochemistry. Rotation (-).



CM 2

CRN 64-18-6

CMF C H2 O2

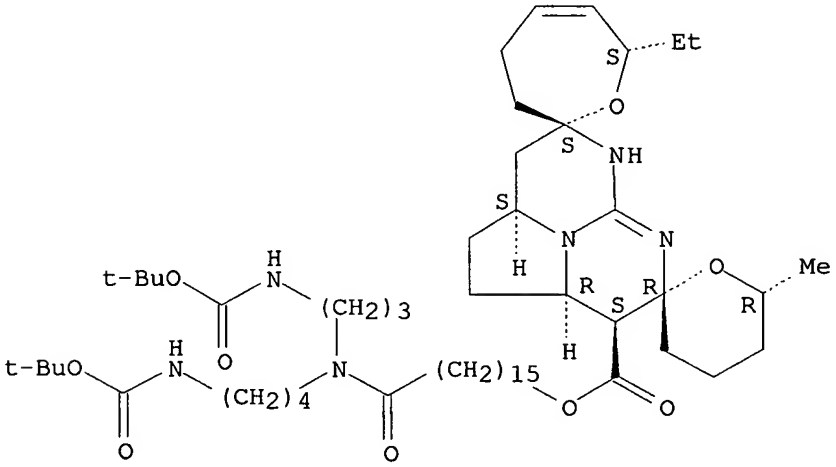


RN 162145-92-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

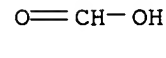
CRN 162145-91-7
CMF C55 H96 N6 O9

Absolute stereochemistry. Rotation (-).



CM 2

CRN 64-18-6
CMF C H2 O2

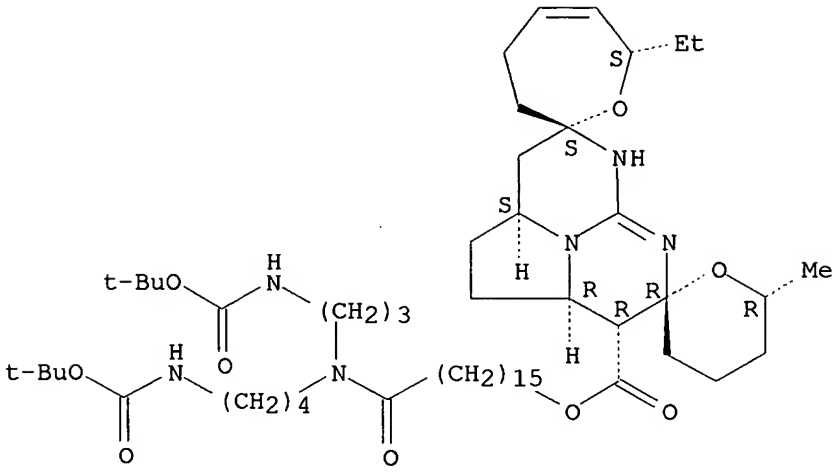


RN 162240-64-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'R,8'aR)-, monoformate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 162240-63-3
CMF C55 H96 N6 O9

Absolute stereochemistry. Rotation (+).

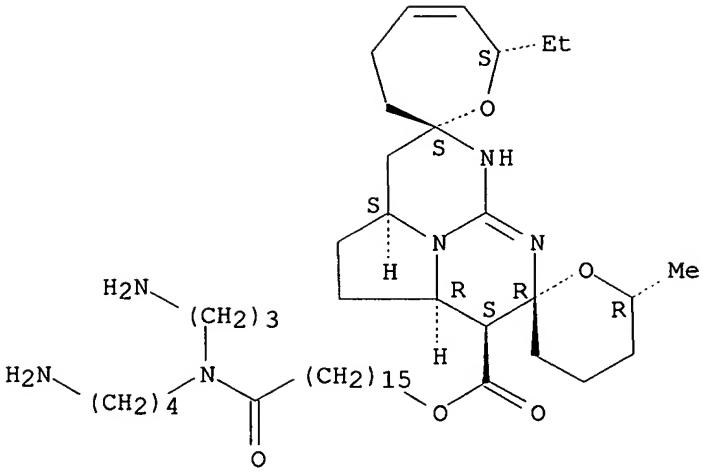


CM 2

CRN 64-18-6
CMF C H2 O2

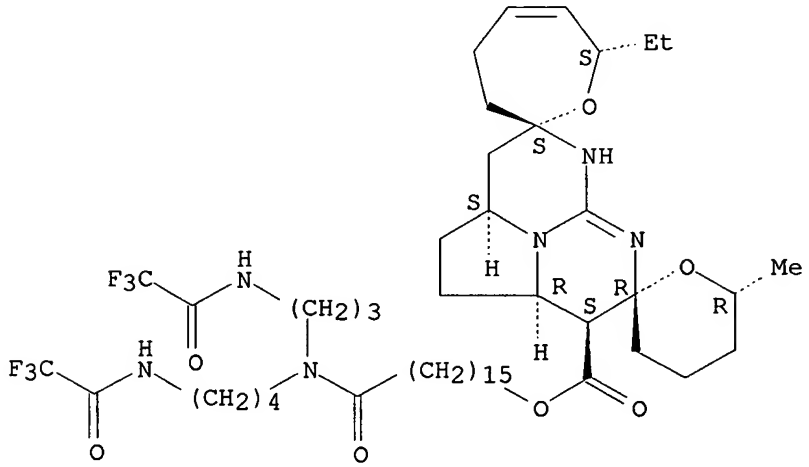
IT 124512-47-6P, (-)-Ptilomycalin A 125422-22-2P
163181-58-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total synthesis of ptilomycalin A)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



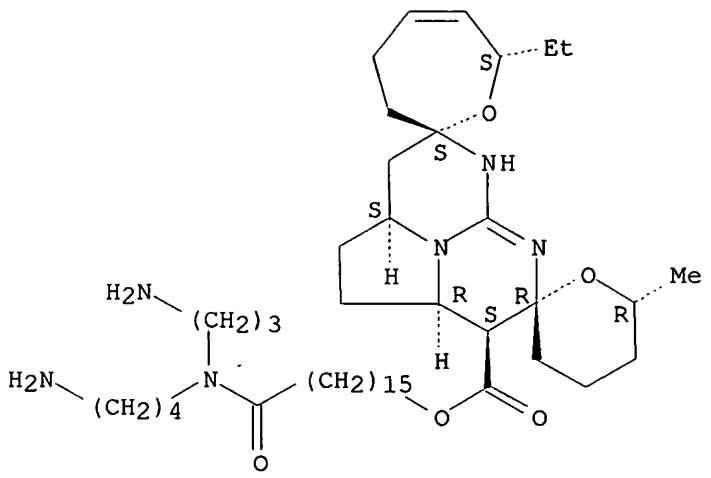
RN 125422-22-2 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[4-[(trifluoroacetyl)amino]butyl][3-[(trifluoroacetyl)amino]propyl]amino]hexadecyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β,8'aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 163181-58-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, monohydrochloride, [2'aS-[2'aα,4'α(R*),7'.alpha.(S*),8'β,8'aα]]- (9CI) (CA INDEX NAME)

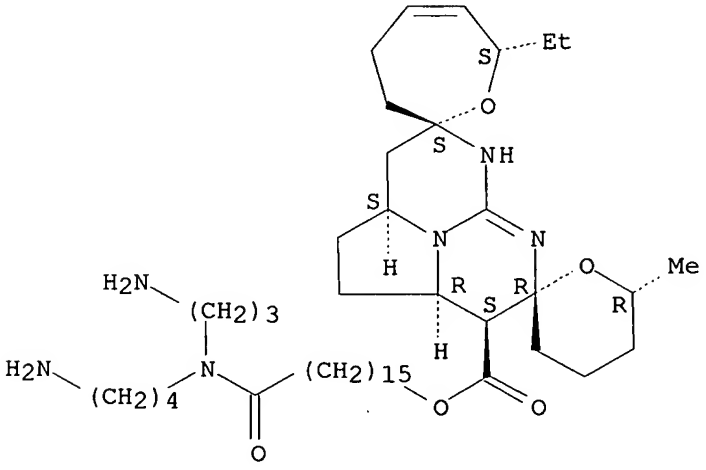
Absolute stereochemistry. Rotation (-).



● HCl

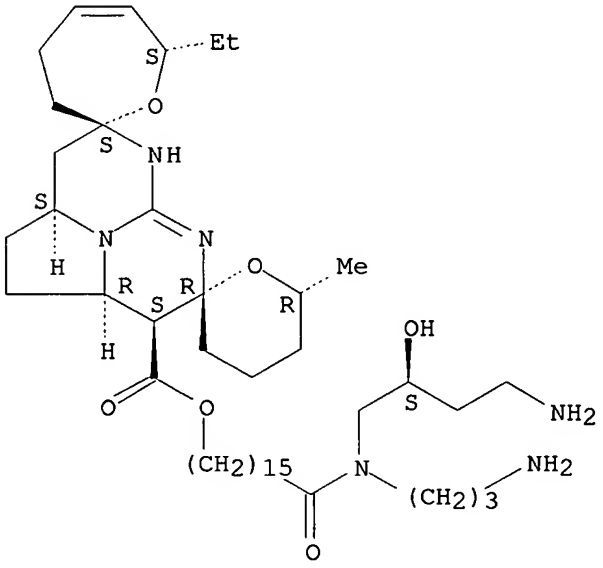
L11 ANSWER 45 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:169849 CAPLUS
DN 122:10342
TI Total syntheses of (±)-chondrillin, (±)-plakorin, and related peroxy ketals. Development of a general route to 3,6-dihydro-1,2-dioxin-3-ols, and, biomimetic syntheses of (±)-crambines A, B, C1, and C2. Revision of the structures of crambines B and C1, and, biomimetic synthesis of the pentacyclic nucleus of ptilomycalin A
AU Shi, Zhongping
CS Brandeis Univ., USA
SO (1994) 172 pp. Avail.: Univ. Microfilms Int., Order No. DA9417716
From: Diss. Abstr. Int. B 1994, 55(3), 908
DT Dissertation
LA English
AB Unavailable
IT 124512-47-6P, Ptilomycalin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(biomimetic synthesis)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

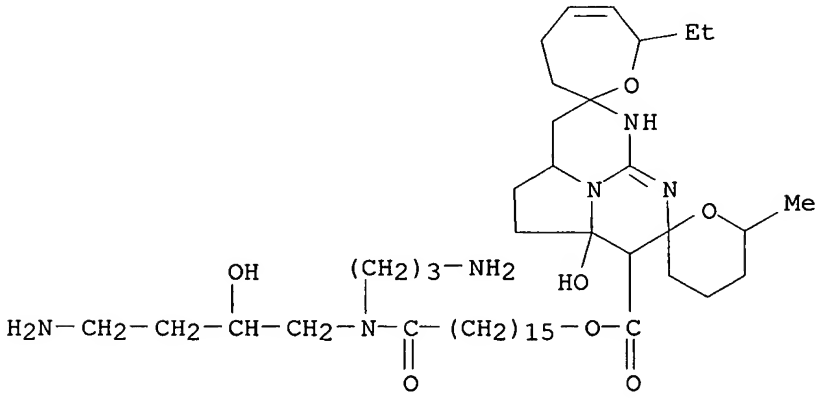


L11 ANSWER 46 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:575634 CAPLUS
DN 121:175634
TI Isolation of Crambescidin 800 from Monanchora arbuscula (Porifera)
AU Tavares, R.; Daloze, D.; Braekman, J. C.; Hajdu, E.; Muricy, G.; Van Soest, R. W. M.
CS Fac. Sciences, Univ. Brussels, Brussels, 1050, Belg.
SO Biochemical Systematics and Ecology (1994), 22(6), 645-6
CODEN: BSECBU; ISSN: 0305-1978
DT Journal
LA English
AB The occurrence in M. arbuscula of crambescidin 800 and of crambescin-type derivs. that are also present in Crambe crambe, supports a close relationship between these 2 genera.
IT 135257-46-4, Crambescidin 800
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, taxonomy in relation to)
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

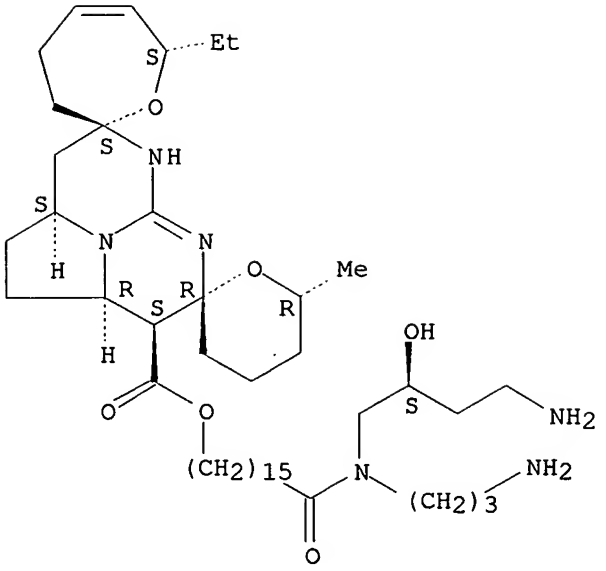


L11 ANSWER 47 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:575530 CAPLUS
DN 121:175530
TI Chromatographic approach to polar compounds: isolation of hydrophilic constituents of the marine sponge Crambe crambe
AU Berlinch, Roberto Gomes de Souza
CS Inst. Fis. Quim., Univ. Sao Paulo, Sao Carlos, 13560-970, Brazil
SO Quimica Nova (1994), 17(2), 167-71
CODEN: QUNODK; ISSN: 0100-4042
DT Journal
LA English
AB The separation steps utilized for the isolation of the constituents of the marine sponge Crambe crambe polar exts. are discussed in detail. Many members of the crambescidine family and its homologs were isolated.
IT 135257-45-3, Crambescidine 816 135257-46-4, Crambescidine 800 151121-78-7
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge)
RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



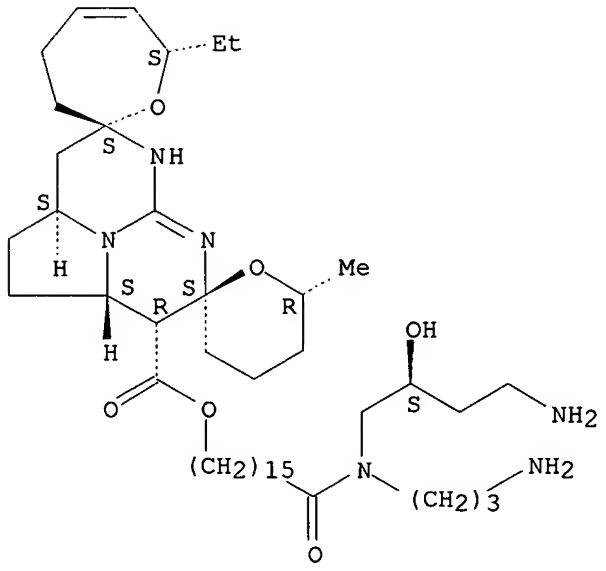
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



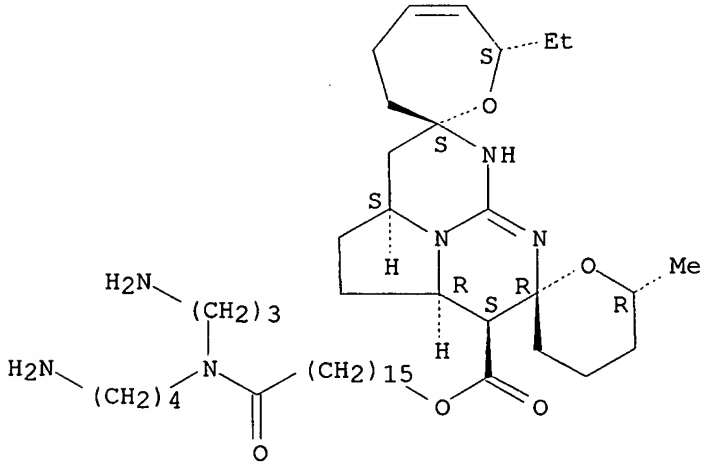
RN 151121-78-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



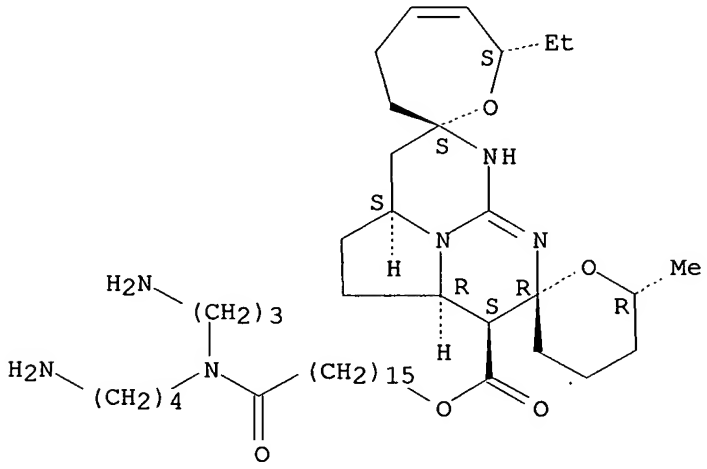
L11 ANSWER 48 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:533825 CAPLUS
DN 121:133825
TI Synthesis of a pentacyclic model of ptilomycalin A
AU Murphy, Patrick J.; Williams, Harri Lloyd
CS Dep. Chem., Univ. Wales, Bangor/Gwynedd, LL57 2UW, UK
SO Journal of the Chemical Society, Chemical Communications (1994), (7), 819-20
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB The conversion of dienes I (n = 4, 5) into the pentacyclic guanidine compds. II (m = 1, 2) is reported; their preparation illustrates a potentially biomimetic synthetic route to the biol. active natural product ptilomycalin A.
IT 124512-47-6, Ptilomycalin A
RL: RCT (Reactant); RACT (Reactant or reagent)
(pentacyclic model fragment for, preparation of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



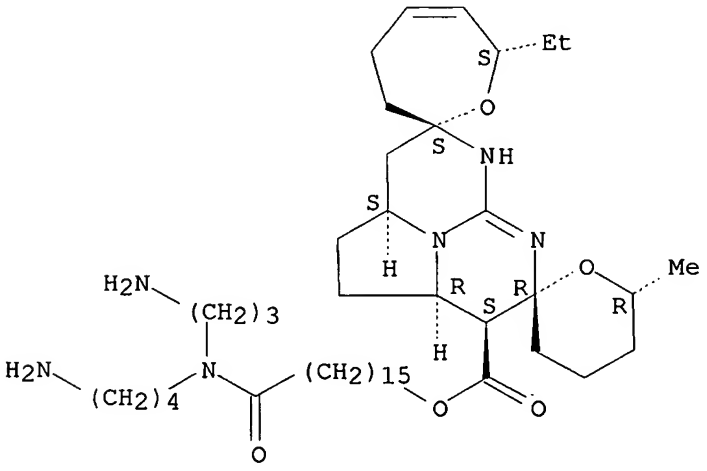
L11 ANSWER 49 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:457763 CAPLUS
DN 121:57763
TI Studies toward the synthesis of ptilomycalin A analogs
AU Grillot, Anne Laure
CS Ohio State Univ., Columbus, OH, USA
SO (1993) 449 pp. Avail.: Univ. Microfilms Int., Order No. DA9411957
From: Diss. Abstr. Int. B, 1994, 54(11), 5666
DT Dissertation
LA English
AB Unavailable
IT 124512-47-6DP, Ptilomycalin A, analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



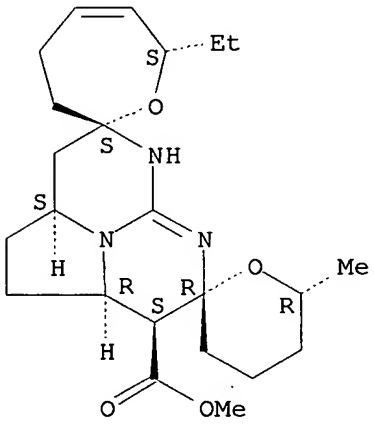
L11 ANSWER 50 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:299058 CAPLUS
DN 120:299058
TI Synthetic studies towards ptilomycalin A using a biomimetic approach
AU Murphy, Patrick J.; Williams, Harri Lloyd; Hursthouse, Michael B.; Abdul Malik, K. M.
CS Dep. Chem., Univ. Wales, Bangor/Gwynedd, LL57 2UW, UK
SO Journal of the Chemical Society, Chemical Communications (1994), (1), 119-20
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB Two model compds., the tetracycle I and the tricycle II are prepared using a biomimetic synthetic approach to the guanidine-containing natural product ptilomycalin A (III).
IT 124512-47-6P, Ptilomycalin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(pyrrolopyrimidopyrimidine spiropyranpyrrolopyrimidopyrimidine fragments of, preparation of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



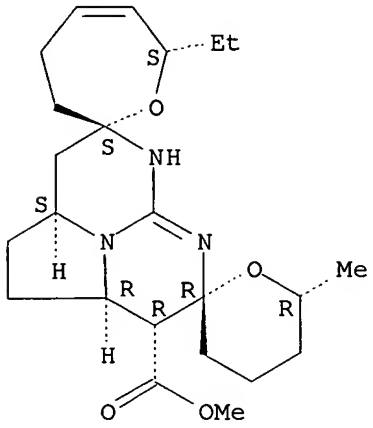
L11 ANSWER 51 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:270940 CAPLUS
DN 120:270940
TI Biomimetic synthesis of the pentacyclic nucleus of ptilomycalin A
AU Snider, Barry B.; Shi, Zhongping
CS Dep. Chem., Brandeis Univ., Waltham, MA, 02254, USA
SO Journal of the American Chemical Society (1994), 116(2), 549-57
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CASREACT 120:270940
AB The Me ester of the pentacyclic nucleus of ptilomycalin A (I) has been prepared by an efficient, convergent, biogenetic, 14-step route. The key steps involve the conversion of acyclic bis enone II (R = Me3CSiPh2) to I in four steps. Michael addition of O-methylisourea to II afforded 52% of a mixture of isoureas, which were both converted to 72% of tricyclic animals III by ammonolysis. Deprotection of the silyl ethers with HF and cyclization with Et3N in MeOH afforded I (≈34% from III) and the diastereomer with an equatorial Me ester group (≈26% from III).
IT 147664-31-1P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(biomimetic synthesis of)
RN 147664-31-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β,8'aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

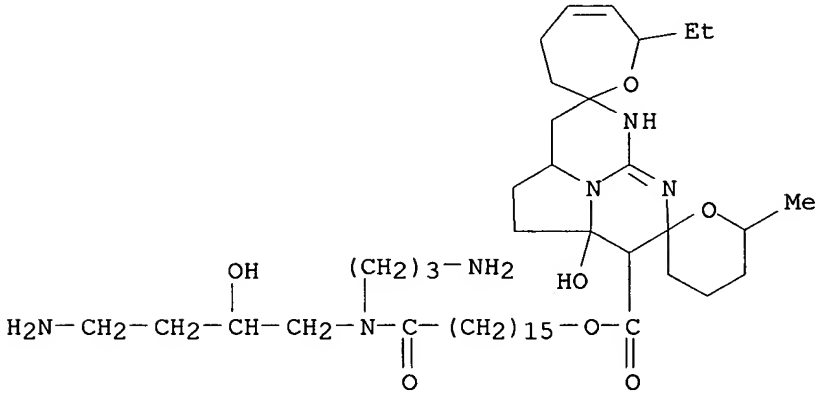


IT 154631-67-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 154631-67-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'α,8'aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

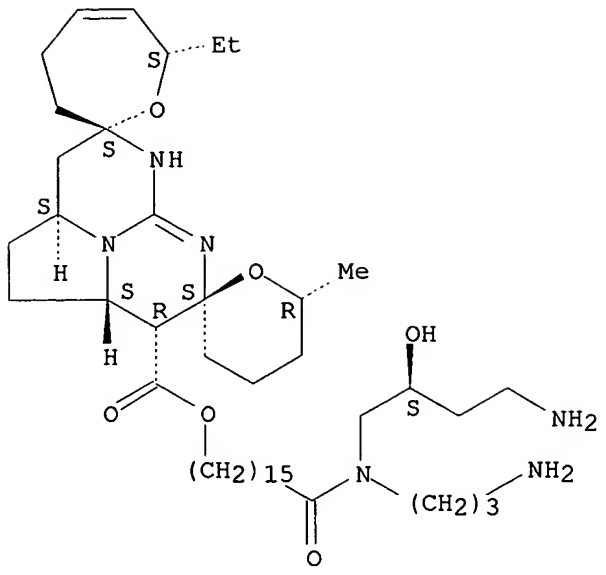


L11 ANSWER 52 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:649766 CAPLUS
DN 119:249766
TI Polycyclic guanidine-containing compounds from the Mediterranean sponge Crambe crambe: the structure of 13,14,15-isocrambescidin 800 and the absolute stereochemistry of the pentacyclic guanidine moieties of the crambescidins
AU Jares-Erijman, Elizabeth A.; Ingrum, April L.; Carney, John R.; Rinehart, Kenneth L.; Sakai, Ryuichi
CS Roger Adams Lab., Univ. Illinois, Urbana, IL, 61801, USA
SO Journal of Organic Chemistry (1993), 58(18), 4805-8
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
AB The absolute stereochem. of the pentacyclic guanidine moieties of crambescidin 816 (I) and of 13,14,15-isocrambescidin 800 (II), a new member of this family, were determined, based on chiral GC anal. of a derivative of 2-hydroxybutanoic acid, an ozonolysis product of the crambescidins. Significantly less antiviral activity and cytotoxicity were observed for II than form other crambescidins.
IT 135257-45-3, Crambescidin 816 151121-78-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(absolute configuration of guanidine moiety of)
RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)

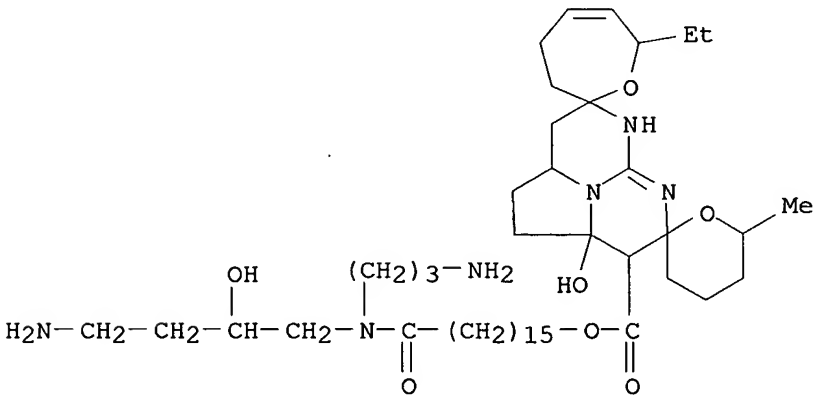


RN 151121-78-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

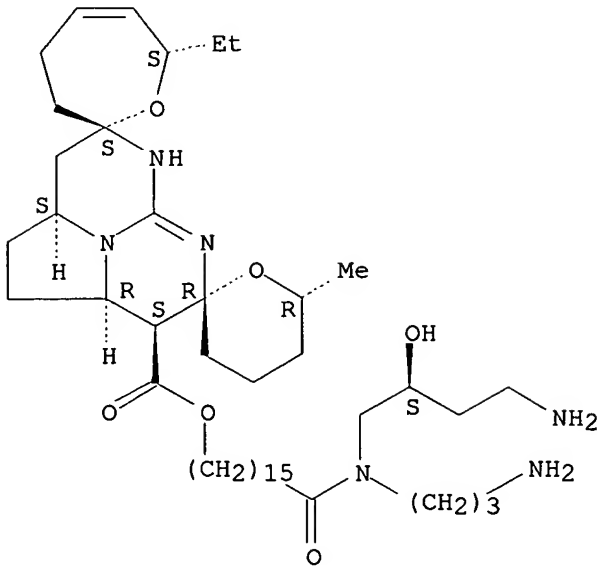

Et
S
O
S
NH
S
N
N
H
S
S
O
Me
R
R
H
OH
S
NH2
O
O
(CH2)15
N
NH2
(CH2)3
O

L11 ANSWER 53 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:646144 CAPLUS
DN 119:246144
TI Polycyclic guanidine alkaloids from the marine sponge Crambe crambe and calcium channel blocker activity of crambescidin 816
AU Berlinck, R. G. S.; Braekman, J. C.; Daloze, D.; Bruno, I.; Riccio, R.; Ferri, S.; Spampinato, S.; Speroni, E.
CS Fac. Sci., Univ. Brussels, Brussels, 1050, Belg.
SO Journal of Natural Products (1993), 56(7), 1007-15
CODEN: JNPRDF; ISSN: 0163-3864
DT Journal
LA English
AB Four pentacyclic guanidine derivs. [crambescidin 800 (I), crambescidin 816 (II), isocrambescidin 800 (III), and crambidine (IV), related to ptilomycalin A] have been isolated from the Mediterranean sponge C. crambe. III and IV are new derivs., the structures of which have been determined on the basis of their spectral properties. The absolute configuration of II at the stereogenic center C-43 has been determined by applying Mosher's method. Pharmacol. and biol. activities of the Crambe crambe alkaloids are reported. In particular, II was found to have a potent Ca2+ antagonist effect and to inhibit the acetylcholine-induced contraction of guinea pig ileum at very low concns.
IT 135257-45-3, Crambescidin 816 135257-46-4, Crambescidin 800 151121-78-7, Isocrambescidin 800
RL: BIOL (Biological study)
(isolation and biol. and pharmacol. activity of, from marine sponge)
RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



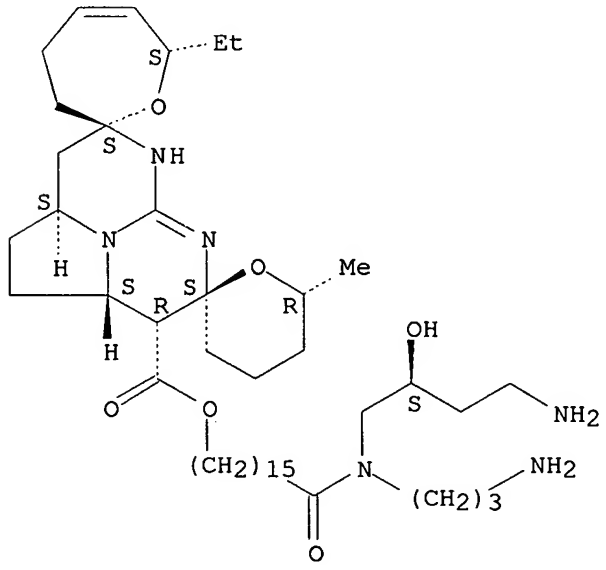
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



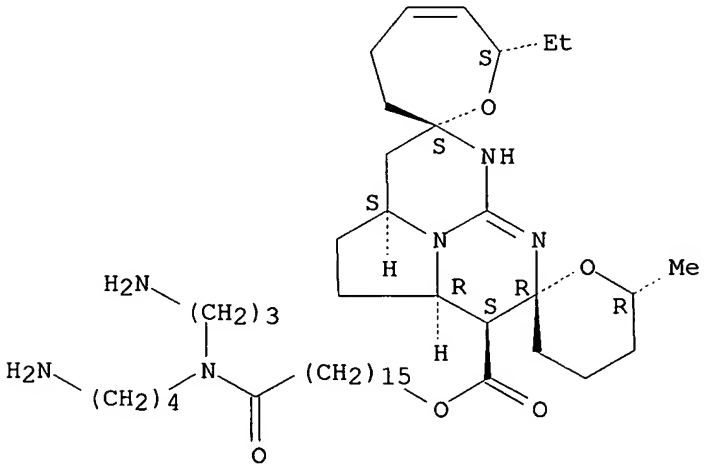
RN 151121-78-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



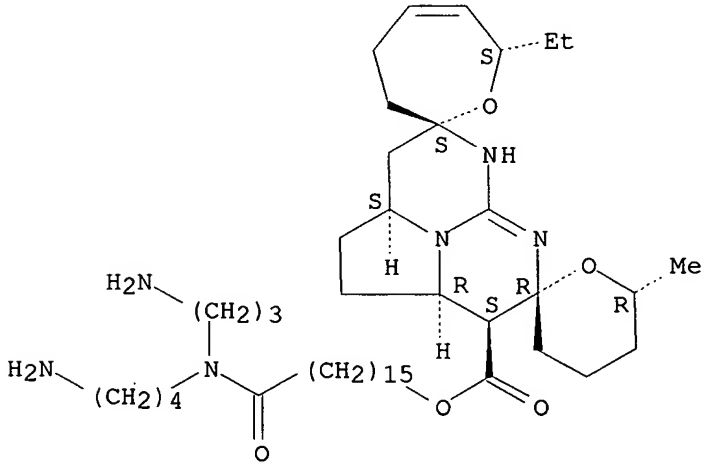
L11 ANSWER 54 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:495899 CAPLUS
DN 119:95899
TI Studies toward the total synthesis of (+)-ptilomycalin A. Use of a tethered Biginelli condensation for the preparation of an advanced tricyclic intermediate
AU Overman, Larry E.; Rabinowitz, Michael H.
CS Dep. Chem., Univ. California, Irvine, CA, 92717-2025, USA
SO Journal of Organic Chemistry (1993), 58(12), 3235-7
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 119:95899
AB The spirotricycle I, a potential intermediate for the enantioselective total synthesis of ptilomycalin A, is prepared in high enantiomeric purity in seven steps from the known β-hydroxy ester (S)-MeO2CCH2CH(OH)CH2CH2CH:CMe2 and nine overall steps from Me acetoacetate. The convergent route developed features the first example of an intramol. ureidoaldehyde condensation of (S)-MeO2CCH2CO(CH2)3CHMeOSiMe2CMe3 with (R)-H2NCONHCH(CH2CH2OH)CH2CH2CH:CMe2 to give pyrrolopyrimidine derivative II (termed a tethered Biginelli condensation).
IT 124512-47-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of intermediate for total synthesis of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L11 ANSWER 55 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:495885 CAPLUS
DN 119:95885
TI Biomimetic synthesis of the central tricyclic portion of ptilomycalin A
AU Snider, Barry B.; Shi, Zhongping
CS Dep. Chem., Brandeis Univ., Waltham, PA, 02254, USA
SO Tetrahedron Letters (1993), 34(13), 2099-102
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 119:95885
AB The central tricyclic portion I of ptilomycalin A (II) is formed from bis enone III in two steps. Addition of O-methylisourea in DMF to III affords a mixture of IV that are both converted to a single tricyclic animal I on treatment with NH3 and NH4OAc in methanol at reflux.
IT 124512-47-6P, Ptilomycalin A
RL: PREP (Preparation)
(biomimetic synthesis of central tricyclic portion of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

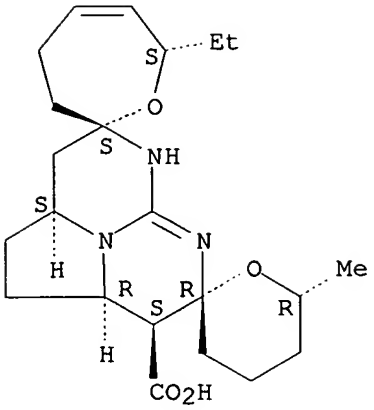


L11 ANSWER 56 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:225662 CAPLUS
DN 118:225662
TI Marine sponge Batzella polycyclic guanidine alkaloid compounds as HIV virus inhibitors
IN Mai, Shing Huey; Nagulapalli, Vasant Kumar; Patil, Ashok D.; Truneh, Alemseged; Westley, John W.
PA SmithKline Beecham Corp., USA
SO PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9301193	A1	19930121	WO 1992-US5517	19920630
	W: AU, CA, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
	AU 9223074	A1	19930211	AU 1992-23074	19920630
PRAI	US 1991-727499	A2	19910709		
	WO 1992-US5517	A	19920630		

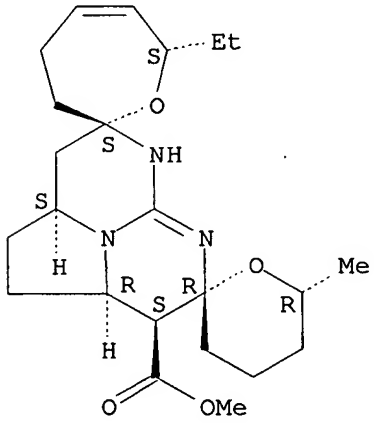
OS MARPAT 118:225662
AB Batzella alkaloids and derivs. (I; R1 = Q; R2 = H, OH, lower alkyl, lower alkenyl, lower alkoxy, aryl, NH2, guanidinyl, etc.; n = 6-10; m = 0, 5-10; dotted line is an optional double bond) or pharmaceutically acceptable salts inhibit infection with the human immunodeficiency virus (HIV). II was purified from Batzella extract and its structure was determined II inhibited binding of HIV glycoprotein gp120 to soluble CD4 antigen in an ELISA and to CD4+ T-cells in a whole cell binding assay with IC50 values of 15 and 10 μM, resp. In a syncytial assay, II had IC50 = 1.7 μg/mL. The cytotoxicity of II against the CD4+ cell line, SupT1, was IC50 = 20 μM. II was derivatized with 2,4-pentanedione to give III, which had IC50 = 5.0 μg/mL in the syncytial assay.
IT 147664-30-0P 147664-31-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from compound from marine sponge Batzella)
RN 147664-30-0 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



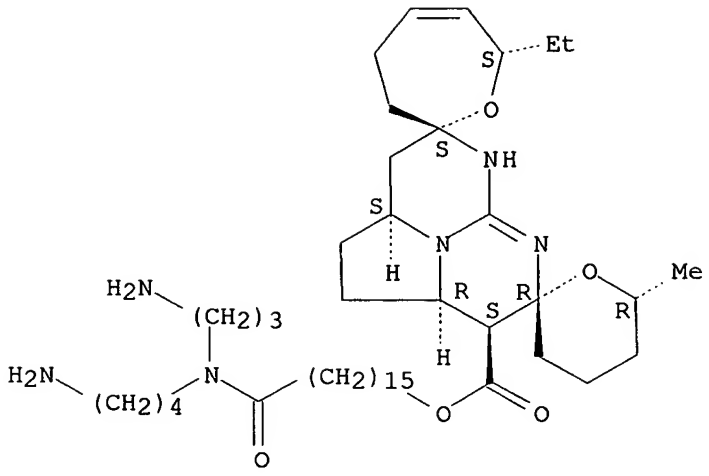
RN 147664-31-1 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, methyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β,8'aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



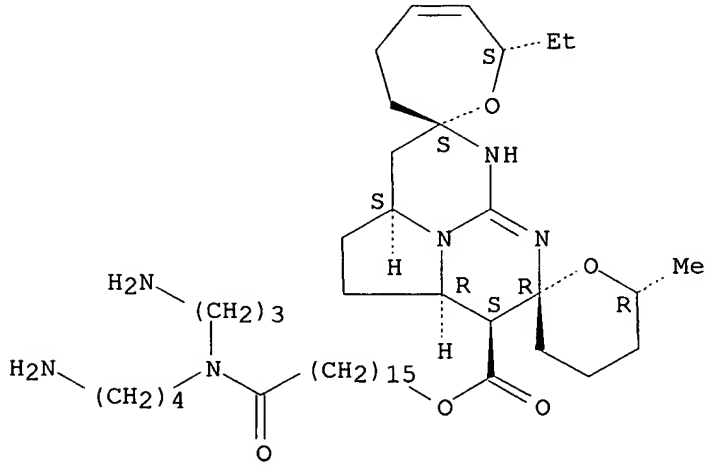
IT 124512-47-6P
RL: PREP (Preparation)
(purification and characterization of, from marine sponge Batzella, as HIV virus inhibitor)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).


Et
S
O
S
NH
S
N
N
H
R
R
O
Me
R
S
H
H2N
(CH2)3
H2N
N
(CH2)15
(CH2)4
O
O
O

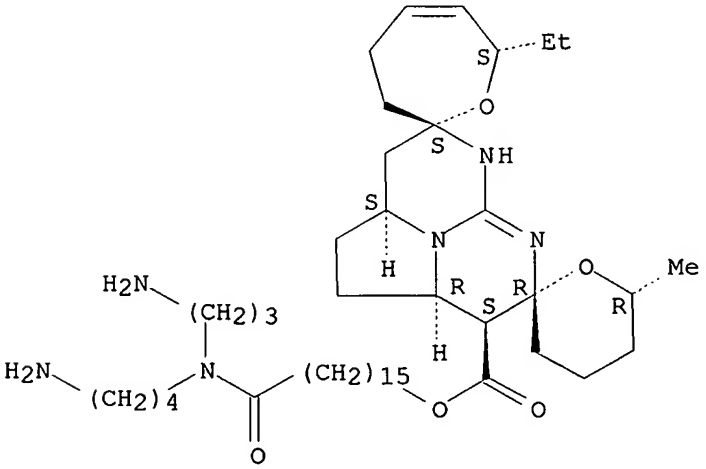
L11 ANSWER 57 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:192079 CAPLUS
DN 118:192079
TI The chemistry of N-sulfinyl compounds and a synthetic approach to ptilomycalin A
AU Alexander, Michael David
CS Pennsylvania State Univ., University Park, PA, USA
SO (1991) 145 pp. Avail.: Univ. Microfilms Int., Order No. DA9214101 From: Diss. Abstr. Int. B 1992, 52(12, Pt. 1), 6388
DT Dissertation
LA English
AB Unavailable
IT 124512-47-6P, Ptilomycalin A
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of, approach to)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L11 ANSWER 58 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1992:592135 CAPLUS
DN 117:192135
TI Structure and chemical properties of ptilomycalin A
AU Ohtani, Ikuko; Kusumi, Takenori; Kakisawa, Hiroshi; Kashman, Yoel; Hirsh, Shulamit
CS Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SO Journal of the American Chemical Society (1992), 114(22), 8472-9
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB The structure of ptilomycalin A (I, R = H) (II) , a marine alkaloid possessing potent antiviral and antibiotic activities, has been determined on the basis of NMR analyses of I (R = F3CCO) (III). It has a unique structure consisting of a polycyclic guanidine and a spermidine group, each of which is linked to a 16-hydroxyhexadecanoic acid moiety. The rotational isomerism of the acylated spermidine moiety was studied by comparing the NMR properties of the synthetic trifluoroacetyl derivs. of spermidine, dipropylenetriamine, diethylenetriamine, and pentylamine. From these expts., a plausible conformation of II and III has been proposed, in which an anion is trapped between the guanidine and spermidine moieties. The III acts as a phase-transfering agent. NMR anal. of the stability of the complexes formed between III and several organic carboxylates in CDCl3 solns. has been carried out.
IT 124512-47-6P
RL: PREP (Preparation)
(from Ptilocaulis spiculifer and Hemimycale, structure of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



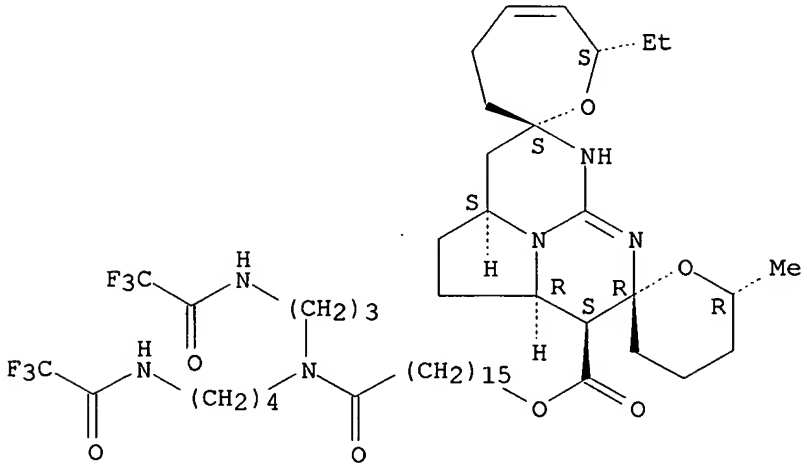
IT 125422-23-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 125422-23-3 CAPLUS

CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[4-[(trifluoroacetyl)amino]butyl][3-[(trifluoroacetyl)amino]propyl]amino]hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

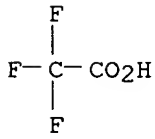
CRN 125422-22-2
CMF C49 H78 F6 N6 O7

Absolute stereochemistry. Rotation (-).



CM 2

CRN 76-05-1
CMF C2 H F3 O2

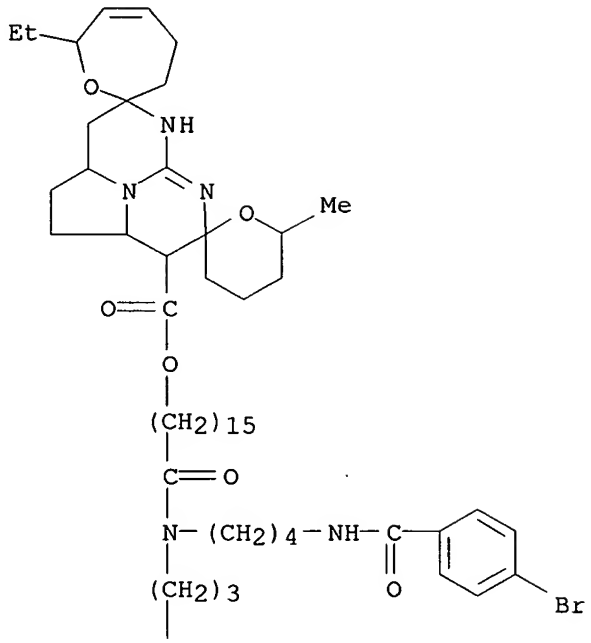


IT 125422-25-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 125422-25-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[(4-bromobenzoyl)amino]butyl][3-[(4-bromobenzoyl)amino]propyl]amino]-16-oxohexadecyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β,8'aα]]-, mono(4-bromobenzoate) (9CI) (CA INDEX NAME)

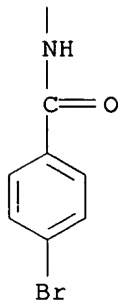
CM 1

CRN 125422-24-4
CMF C59 H86 Br2 N6 O7

PAGE 1-A

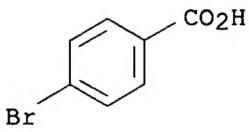


PAGE 2-A



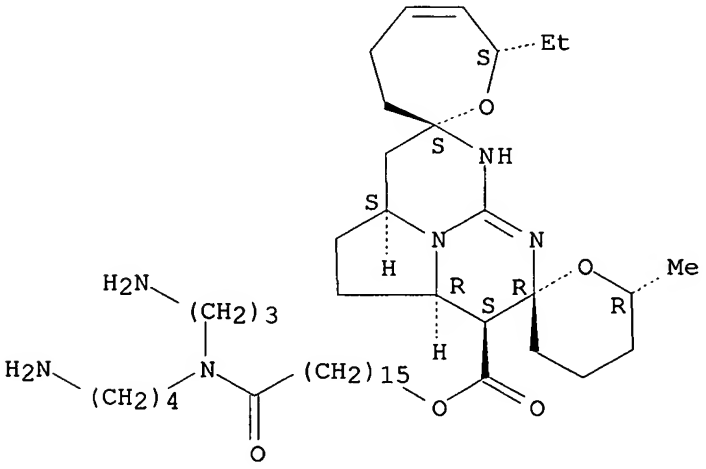
CM 2

CRN 586-76-5
CMF C7 H5 Br O2


CO2H
Br

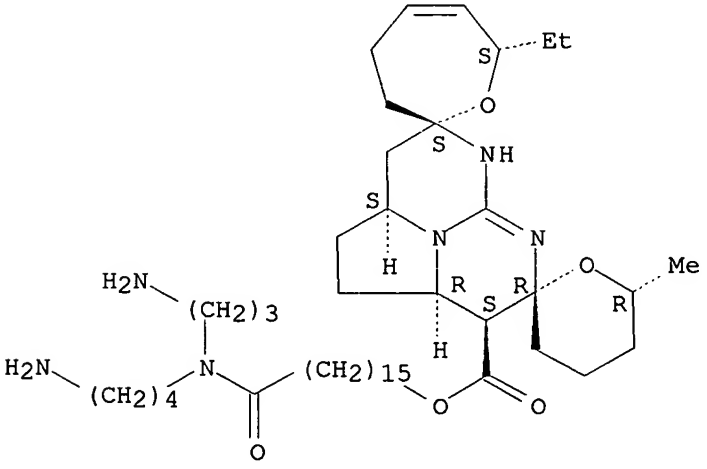
L11 ANSWER 59 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1992:470110 CAPLUS
DN 117:70110
TI An insight into the conformation of ptilomycalin A. The NMR properties of trifluoroacetylated spermidine analogs
AU Ohtani, Ikuko; Kusumi, Takenori; Kakisawa, Hiroshi
CS Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SO Tetrahedron Letters (1992), 33(18), 2525-8
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB The conformation of the bis(trifluoroacetyl) derivative of ptilomycalin A (I), a biol. active marine alkaloid, has been deduced from analyzing the NMR properties of the trifluoroacetyl derivs. of spermidine and its analogs.
IT 124512-47-6, Ptilomycalin A
RL: PRP (Properties)
(conformation of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

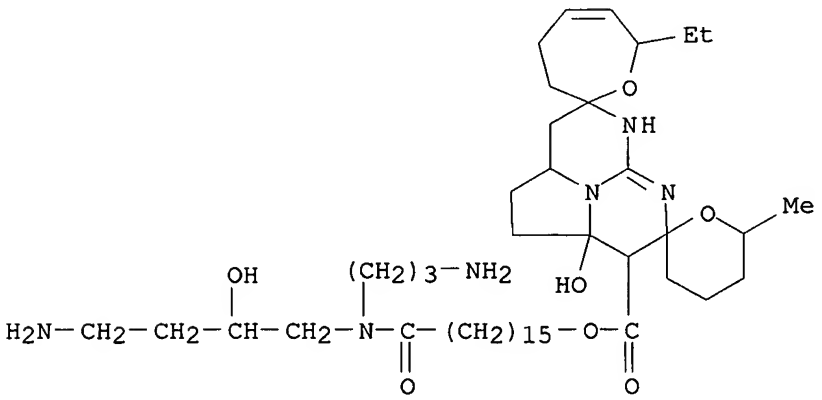


L11 ANSWER 60 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1991:603689 CAPLUS
DN 115:203689
TI Marine alkaloid, ptilomycalin, recognizing anions. Does the ability correlate with its bioactivity?
AU Kusumi, Takenori
CS Inst. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SO Kagaku to Seibutsu (1991), 29(6), 347-8
CODEN: KASEAA; ISSN: 0453-073X
DT Journal; General Review
LA Japanese
AB A review with 2 refs. on ptilomycalin A from sponge of the Red Sea having strong antiviral and antitumor activities. Recognition of amino acid anions by ptilomycalin A trifluoroacetyl derivative is disclosed.
IT 124512-47-6, Ptilomycalin A
RL: BIOL (Biological study)
(anion recognition by, of sponge)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



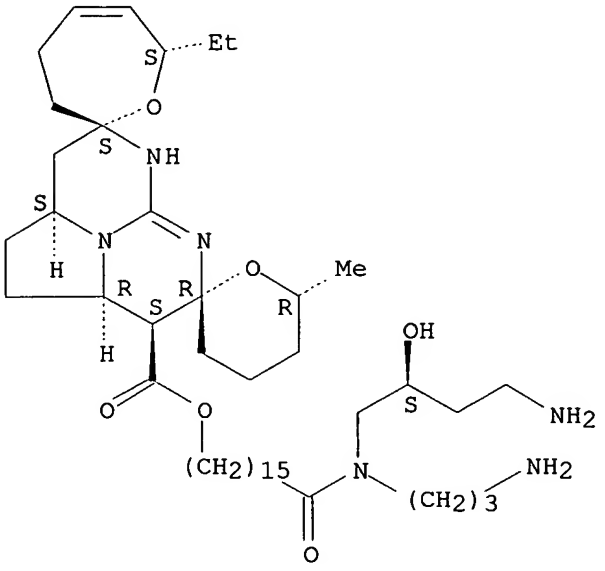
L11 ANSWER 61 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1991:532188 CAPLUS
DN 115:132188
TI Crambescidins: new antiviral and cytotoxic compounds from the sponge Crambe crambe
AU Jares-Erijman, Elizabeth A.; Sakai, Ryuichi; Rinehart, Kenneth L.
CS Roger Adams Lab., Univ. Illinois, Urbana, IL, 61801, USA
SO Journal of Organic Chemistry (1991), 56(19), 5712-15
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
AB Exts. of the red encrusting Mediterranean sponge C. crambe demonstrated cytotoxicity vs. L1210 murine lymphocytic leukemia cells as well as Herpes simplex virus, type 1. The compds. responsible for this activity, crambescidins 816, 830, 844, and 800 (I, II, III, and IV, resp.), have been isolated and shown to consist of a family of complex pentacyclic guanidines linked by a linear ω-hydroxy fatty acid to a hydroxyspermidine. The compds. are related to the recently described ptilomycalin A, isolated from Caribbean Ptilocaulis and Red Sea Hamimycale species.
IT 135257-45-3
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, isolation and mol. structure and antiviral and cytotoxic activity of)
RN 135257-45-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aS)- (9CI) (CA INDEX NAME)



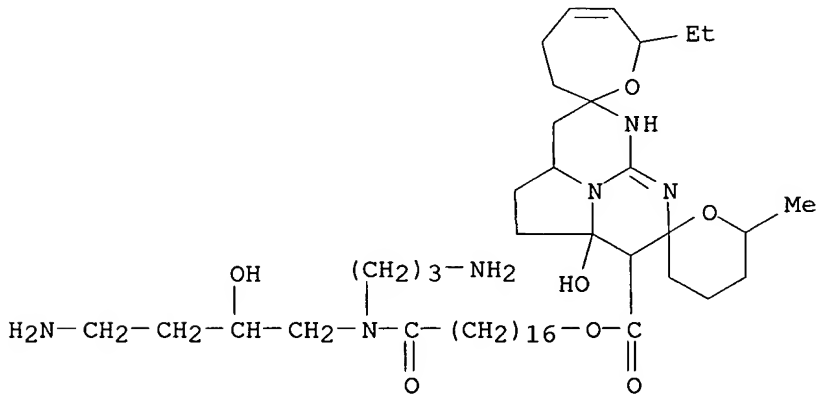
IT 135257-46-4 135257-47-5 135283-73-7
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, isolation and mol. structure and antiviral cytotoxic activity of)
RN 135257-46-4 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[(2S)-4-amino-2-hydroxybutyl](3-

aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-(9CI) (CA INDEX NAME)

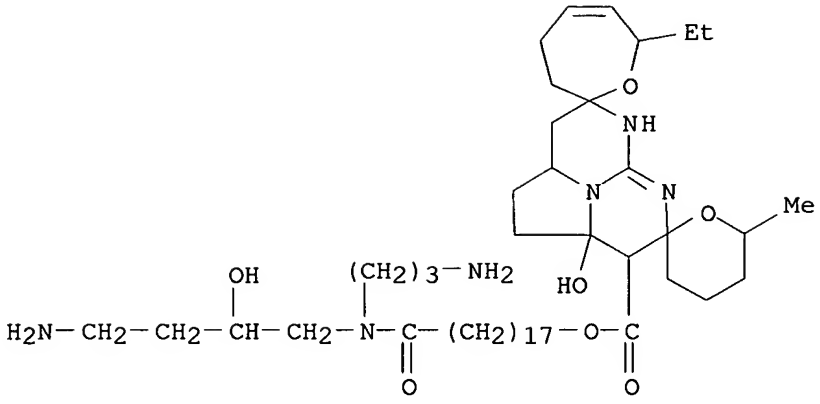
Absolute stereochemistry. Rotation (-).



RN 135257-47-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 17-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-17-oxoheptadecyl ester (9CI) (CA INDEX NAME)



RN 135283-73-7 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-8'a-hydroxy-6''-methyl-, 18-[(4-amino-2-hydroxybutyl)(3-aminopropyl)amino]-18-oxooctadecyl ester (9CI) (CA INDEX NAME)

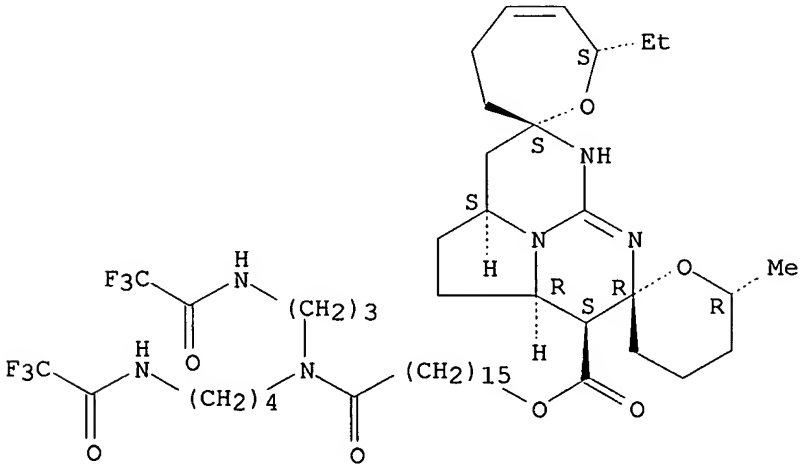

Et
O
NH
N
N
O
Me
HO
OH
(CH2)3—NH2
H2N—CH2—CH2—CH—CH2—N—C—(CH2)17—O—C
O
O

L11 ANSWER 62 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1990:91328 CAPLUS
DN 112:91328
TI Ptilomycalin A. A novel polycyclic guanidine from sponges
AU Ohtani, I.; Kusumi, T.; Kakisawa, H.; Kashman, Y.; Hirsh, S.; McConnell, O. J.
CS Dep. Chem., Univ. Tsukuba, Tsukuba, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1989), 31st, 356-63
CODEN: TYKYDS
DT Journal
LA Japanese
AB In screening for biol. active metabolites from marine sponges, the crude exts. (CHCl3-MeOH, 9:1) of the Caribbean sponge Ptilocaulis spiculifer and the Red Sea sponge Hemimycale species showed a remarkable activity. These exts. were separated by chromatog. to afford the same antitumor, antiviral, and antifungal active compound, ptilomycalin A (I). I has a new carbon skeleton possessing a polycyclic guanidine moiety, which is quite different from those of known guanidino compds. such as tetrodotoxins and saxitoxins. It should be also noted that spermidine is connected with the polycyclic skeleton through an ω-hydroxylated fatty acid.
IT 125422-23-3 125422-25-5
RL: BIOL (Biological study)
(of sponges, as ptilomycalin A metabolite)
RN 125422-23-3 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[4-[(trifluoroacetyl)amino]butyl][3-[(trifluoroacetyl)amino]propyl]amino]hexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

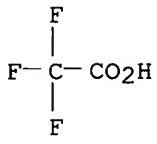
CRN 125422-22-2
CMF C49 H78 F6 N6 O7

Absolute stereochemistry. Rotation (-).



CM 2

CRN 76-05-1
CMF C2 H F3 O2

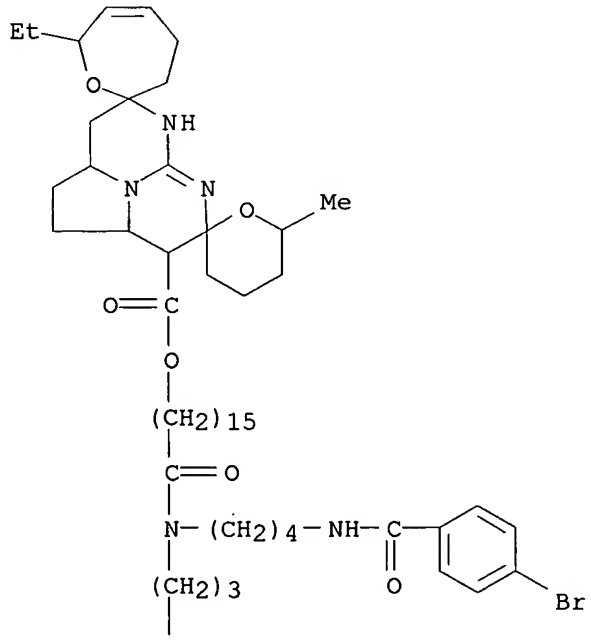


RN 125422-25-5 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[[4-[(4-bromobenzoyl)amino]butyl][3-[(4-bromobenzoyl)amino]propyl]amino]-16-oxohexadecyl ester, [2'aS-[2'aα,4'α(R*),7'α(S*),8'β,8'aα]]-, mono(4-bromobenzoate) (9CI) (CA INDEX NAME)

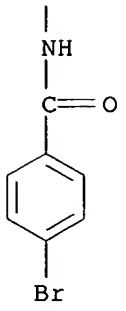
CM 1

CRN 125422-24-4
CMF C59 H86 Br2 N6 O7

PAGE 1-A

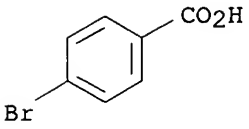


PAGE 2-A



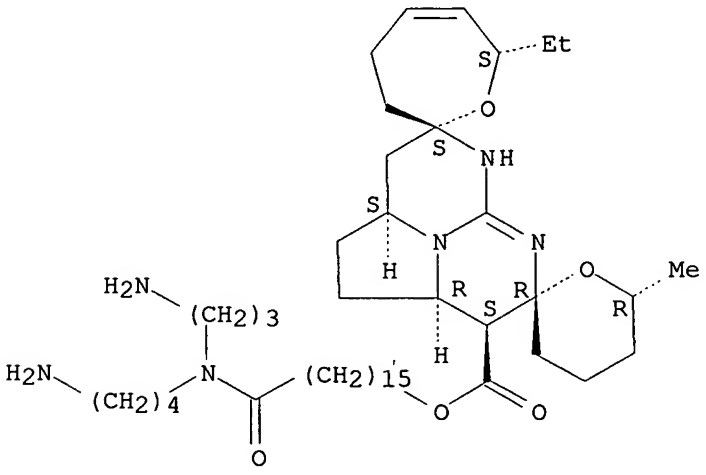
CM 2

CRN 586-76-5
CMF C7 H5 Br O2



IT 124512-47-6
RL: BIOL (Biological study)
(of sponges, structure and biol. activity of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

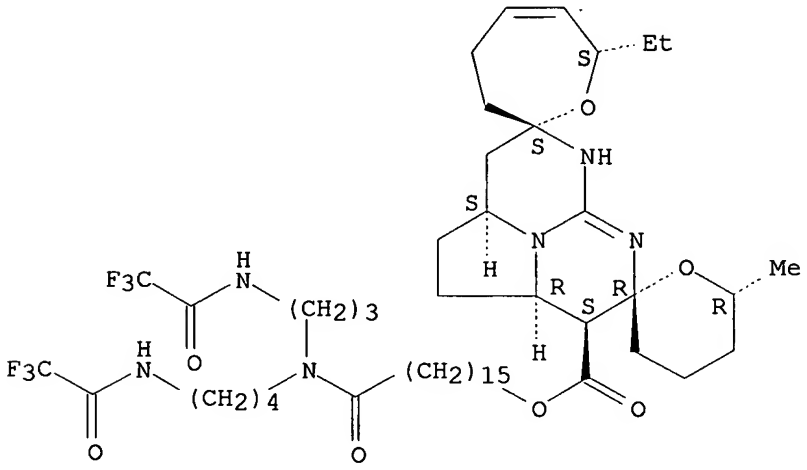


IT 125473-75-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 125473-75-8 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[4-[(trifluoroacetyl)amino]butyl][3-[(trifluoroacetyl)amino]propyl]amino]hexadecyl ester, monomethanesulfonate, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

CM 1

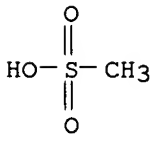
CRN 125422-22-2
CMF C49 H78 F6 N6 O7

Absolute stereochemistry. Rotation (-).



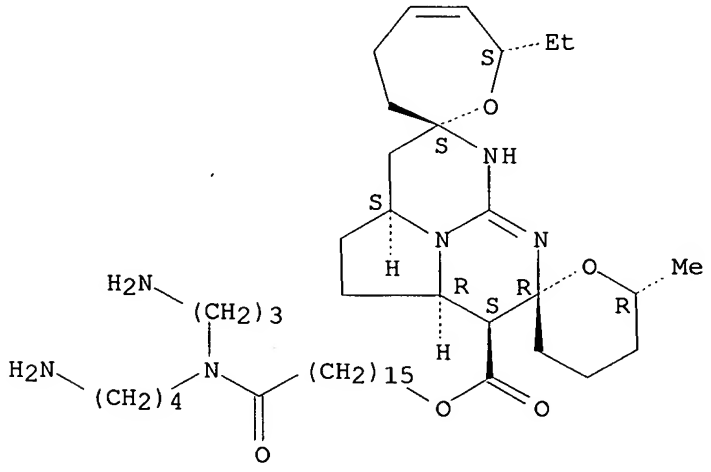
CM 2

CRN 75-75-2
CMF C H4 O3 S



L11 ANSWER 63 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1990:52554 CAPLUS
DN 112:52554
TI Ptilomycalin A: a novel polycyclic guanidine alkaloid of marine origin
AU Kashman, Yoel; Hirsh, Shulamit; McConnell, Oliver J.; Ohtani, Ikuko; Kusumi, Takenori; Kakisawa, Hiroshi
CS Sch. Chem., Tel Aviv Univ., Ramat Aviv, 69978, Israel
SO Journal of the American Chemical Society (1989), 111(24), 8925-6
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB A novel guanidine alkaloid, ptilomycalin A (I), exhibiting remarkable antifungal, antiviral, and antitumor activities, has been isolated from the Caribbean sponge Ptilocaulis spiculifer and the Red Sea sponge Hemimycale. I has a unique polycyclic guanidine moiety connected with a ω-hydroxyhexadecanoylspermidine group through an ester linkage. The structure has been elucidated by spectroscopic analyses and chemical reactions.
IT 124512-47-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, isolation and mol. structure and biol. activity of)
RN 124512-47-6 CAPLUS
CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazaacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-[(4-aminobutyl)(3-aminopropyl)amino]-16-oxohexadecyl ester, (2S,2''R,2'aS,6''R,7S,8'S,8'aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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     FILE 'REGISTRY' ENTERED AT 12:45:20 ON 19 SEP 2006
L1             SCREEN 964 AND 1006 AND 2040
L2             STRUCTURE UPLOADED
L3             QUE L2 AND L1
L4           0 S L3 SSS SAM
L5             STRUCTURE UPLOADED
L6           0 S L5 SSS SAM
L7           0 S L5 SSS FUL
L8             STRUCTURE UPLOADED
L9           9 S L8 SSS SAM
L10        176 S L8 SSS FUL

     FILE 'CAPLUS' ENTERED AT 12:48:40 ON 19 SEP 2006
L11         63 S L10

     FILE 'CAOLD' ENTERED AT 12:49:48 ON 19 SEP 2006

=> s l10
L12          0 L10

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.44     649.54

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00     -42.75

STN INTERNATIONAL LOGOFF AT 12:50:01 ON 19 SEP 2006
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